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Lecture 4 – Clustering

Unsupervised Classification

(Cluster analysis)

Training set is not available, No. of classes may not be *a priori* known

What are clusters?

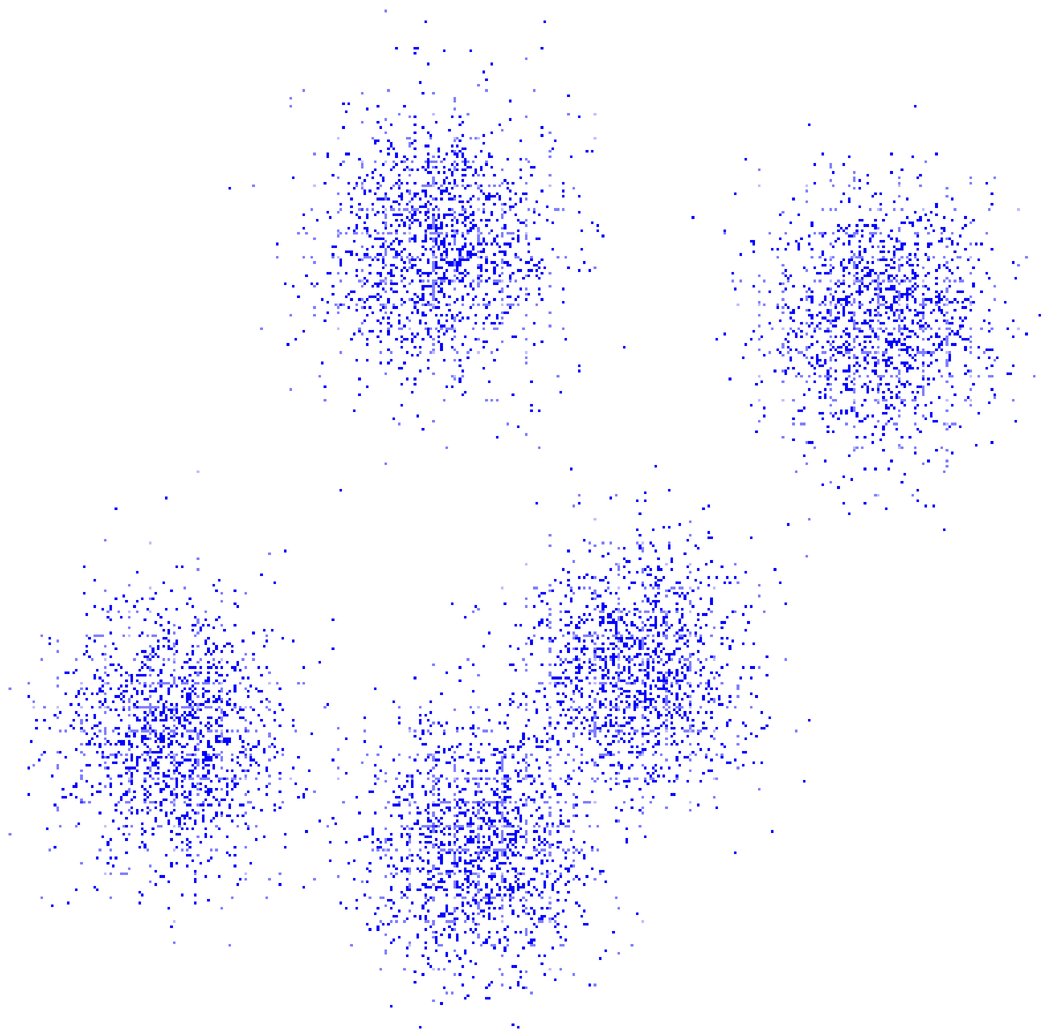
Intuitive meaning

- compact, well-separated subsets

Formal definition

- many attempts, mostly unsatisfactory
  (*t*-connectivity, diameter constraint, ...)
- any partition of the data into disjoint subsets

What are clusters?



How to compare different clusterings? (Ward criterion)

Variance measure J should be minimized

$$J = \sum_{i=1}^{N} \sum_{\mathbf{x} \in C_i} \|\mathbf{x} - \mathbf{m}_i\|^2$$

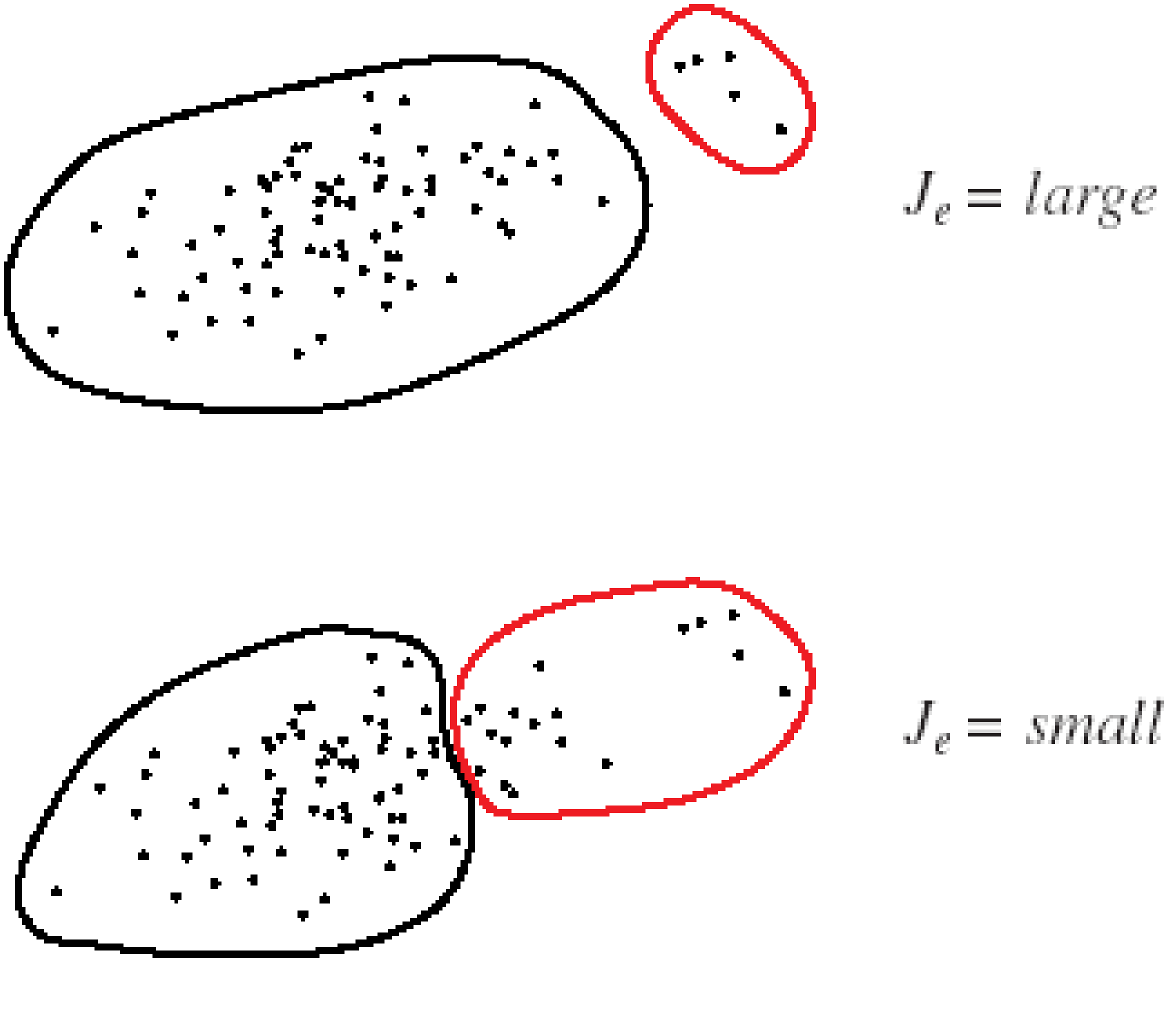
Drawback – only clusterings with the same N can be compared. Global minimum $J = 0$ is reached in the degenerated case.

Minimization of *J*

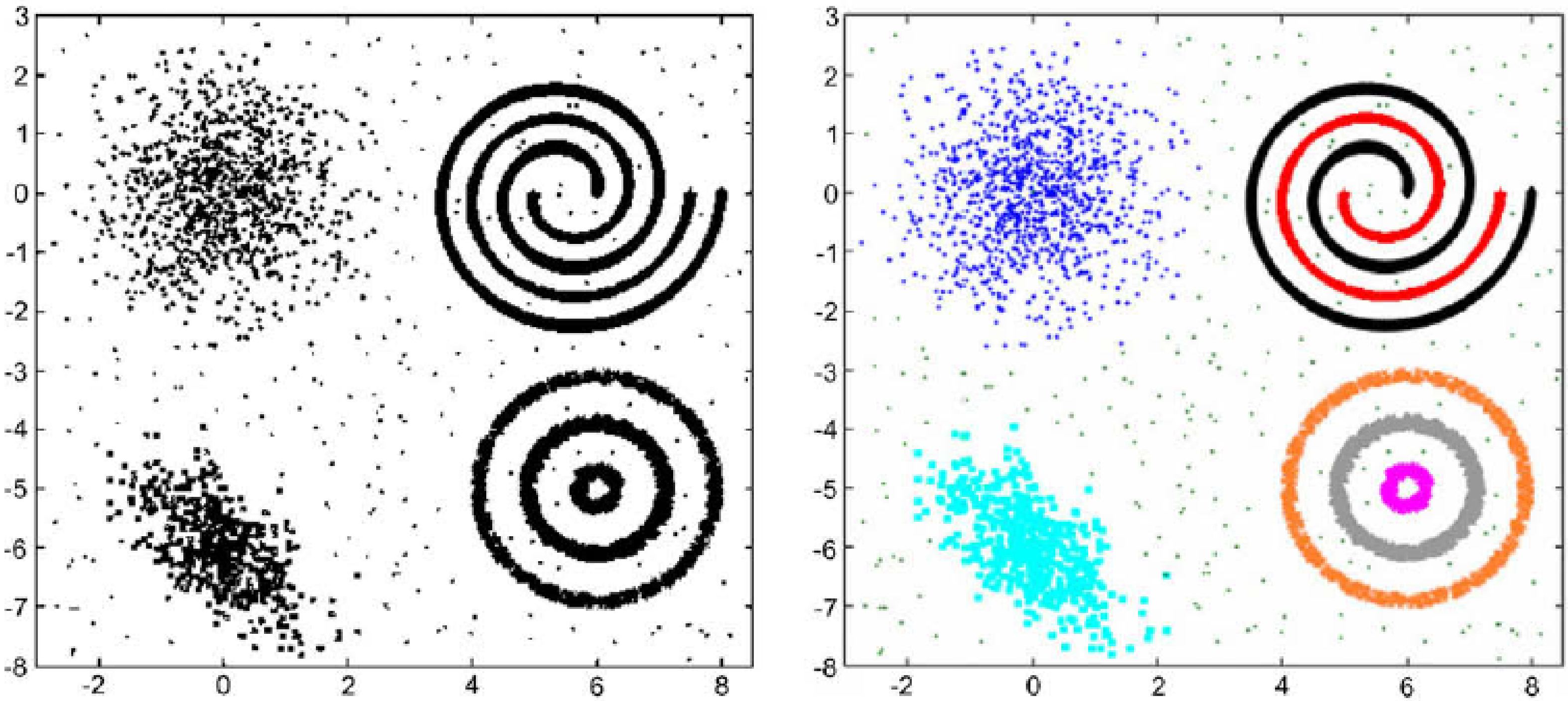
Drawbacks

- The results are sometimes “intuitively wrong” because *J* prefers clusters with approx the same size

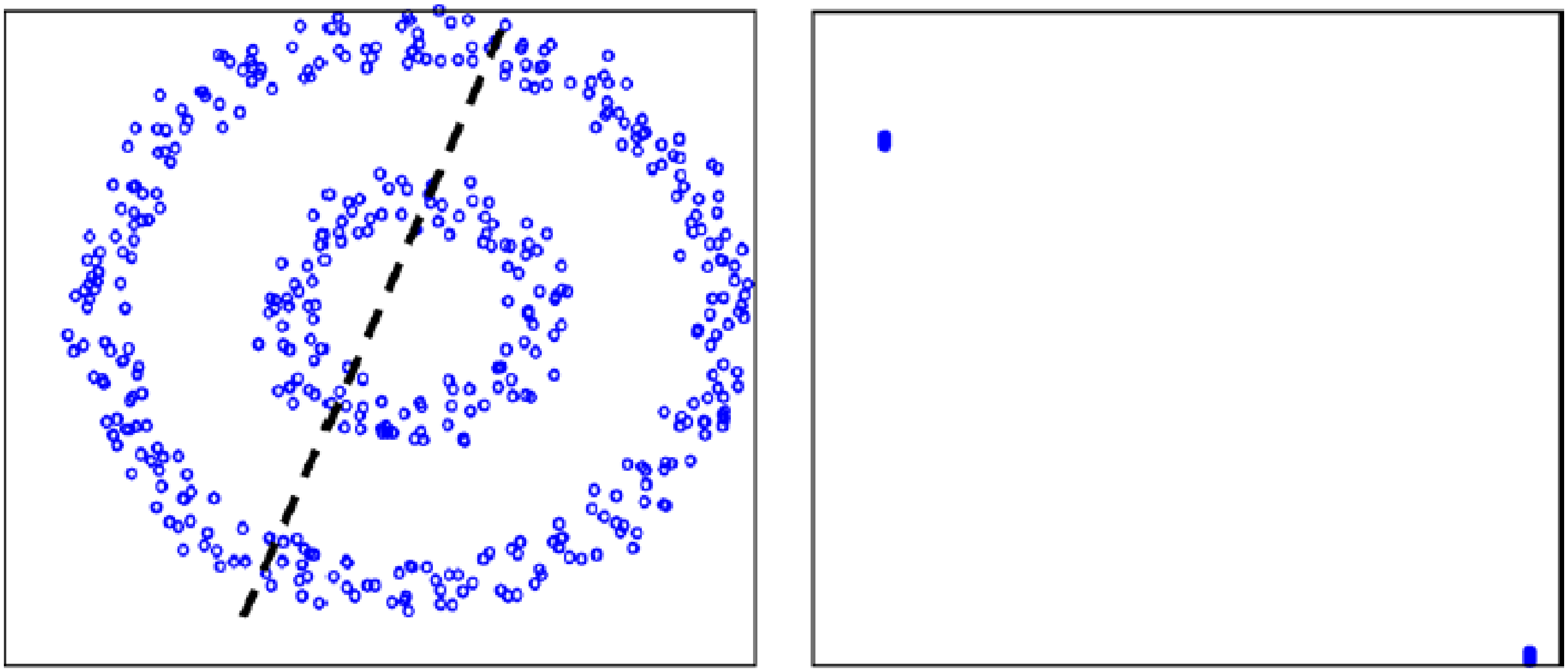
An example of a “wrong” result



Drawback – assumes uncorrelated features and "convex" clusters



Solution – proper transform of the features



Clustering techniques

- **Iterative methods**
  - typically if *N* is given
- **Hierarchical methods**
  - typically if *N* is unknown
- **Other methods**
  - sequential, graph-based, branch & bound, fuzzy, genetic, model-based, etc.

Sequential clustering

- *N* may be unknown
- Very fast but not very good
- Each point is considered only once

Idea: a new point is either added to an existing cluster or it forms a new cluster. The decision is based on the **user-defined distance threshold**.

Sequential clustering

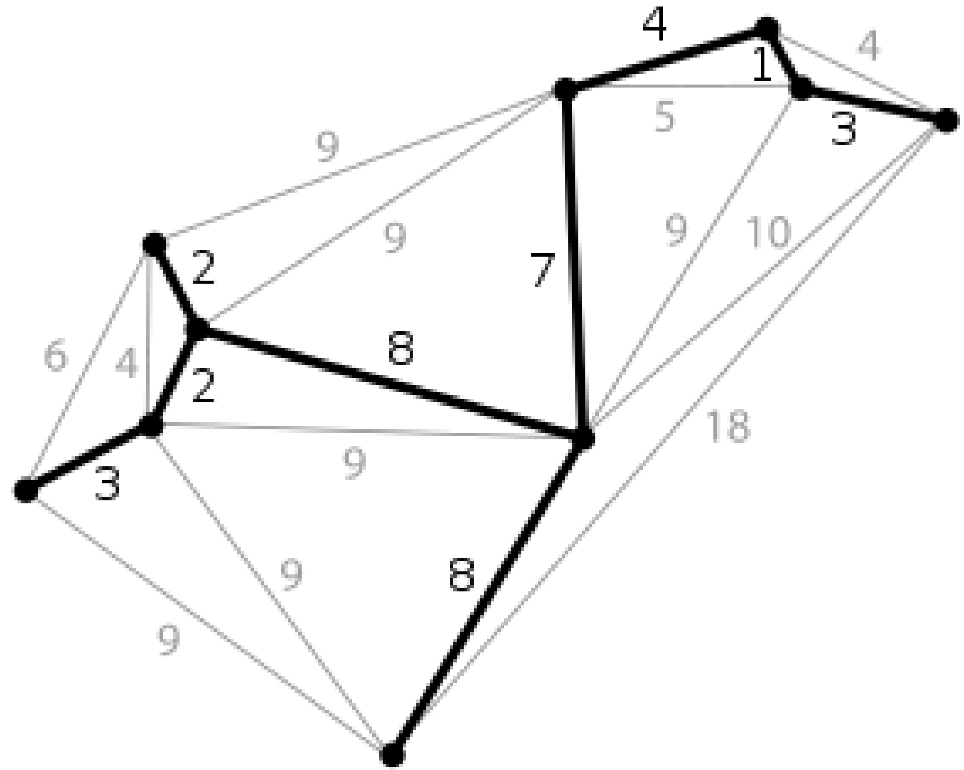
Drawbacks:

- Dependence on the distance threshold
- Dependence on the order of data points

Graph-based clustering

Idea: Construct a shortest spanning tree and then divide it into clusters by removing some edges.

- Naive approach: remove *N*-1 longest edges
- Better: remove *N*-1 long and **inconsistent** edges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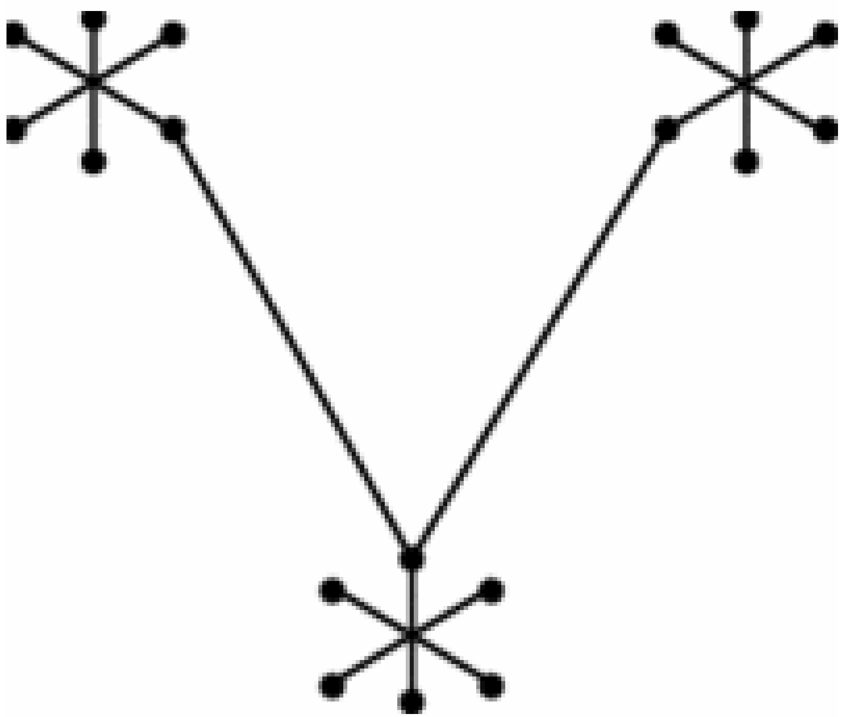


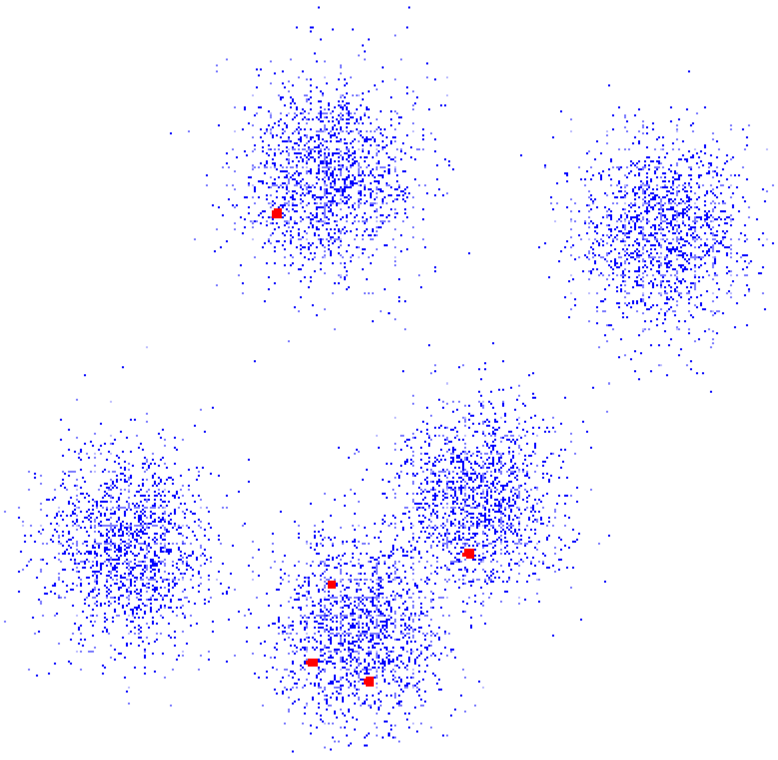
Iterative clustering methods

- ***N*-means clustering**
- **Iterative minimization of *J***
- **ISODATA**

  Iterative Self-Organizing DATa Analysis

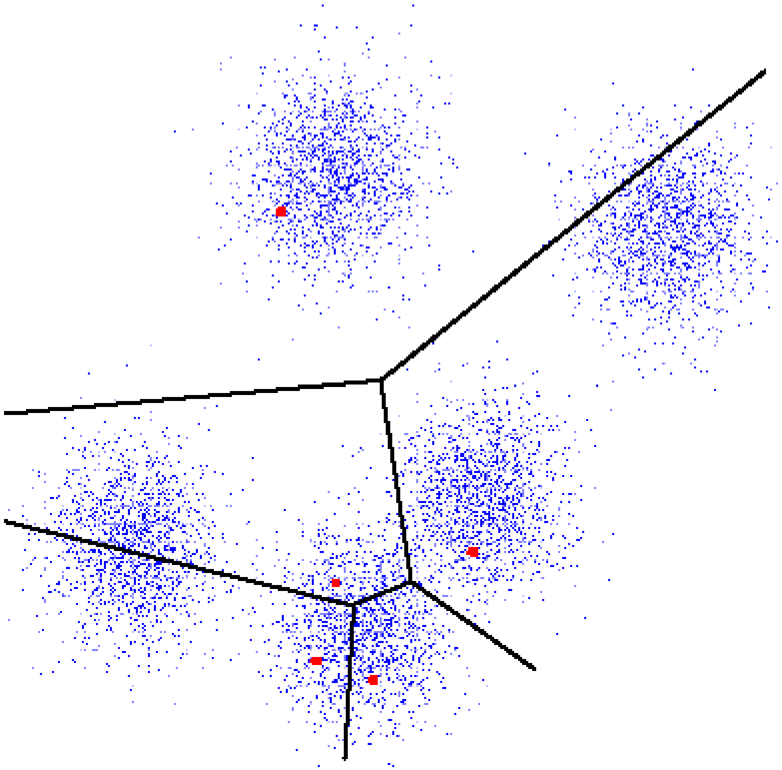
N-means clustering

1. Select *N* initial cluster centroids.



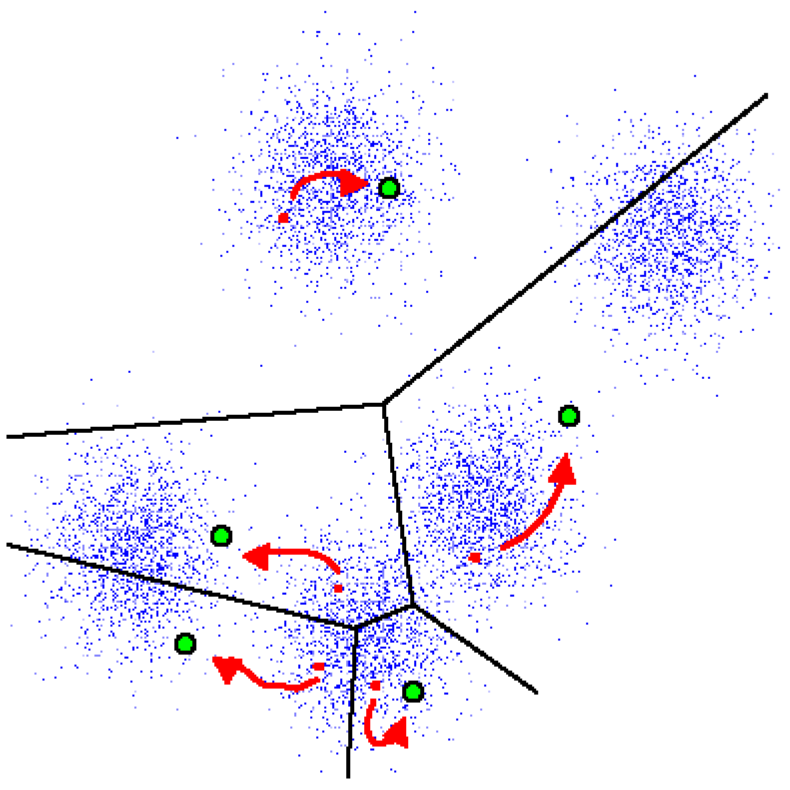
N-means clustering

2. Classify every point *x* according to minimum distance.



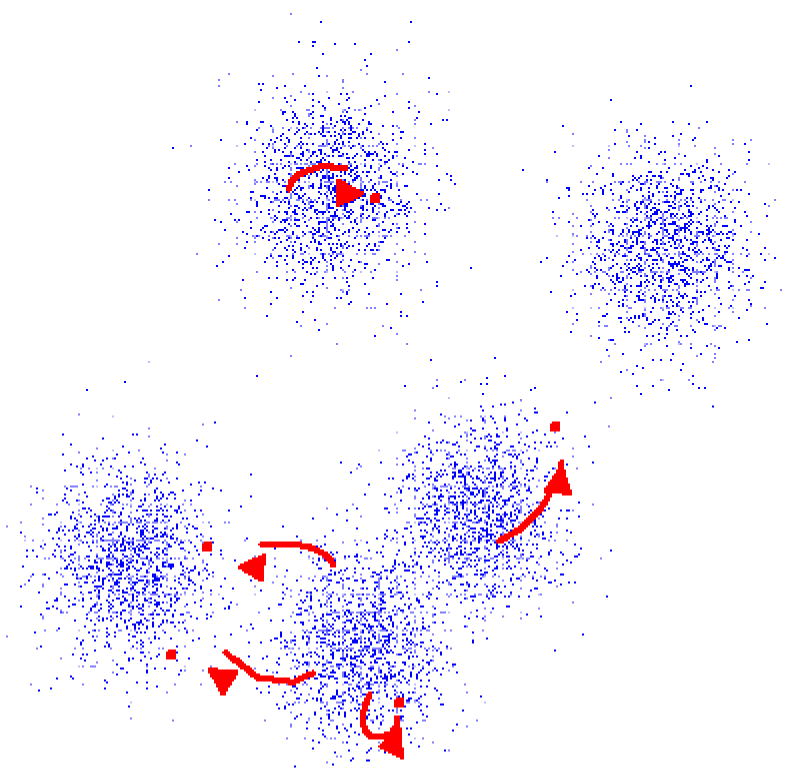
N-means clustering

3. Recalculate the cluster centroids.



N-means clustering

4. If the centroids did not change then STOP else GOTO 2.



N-means clustering

Drawbacks

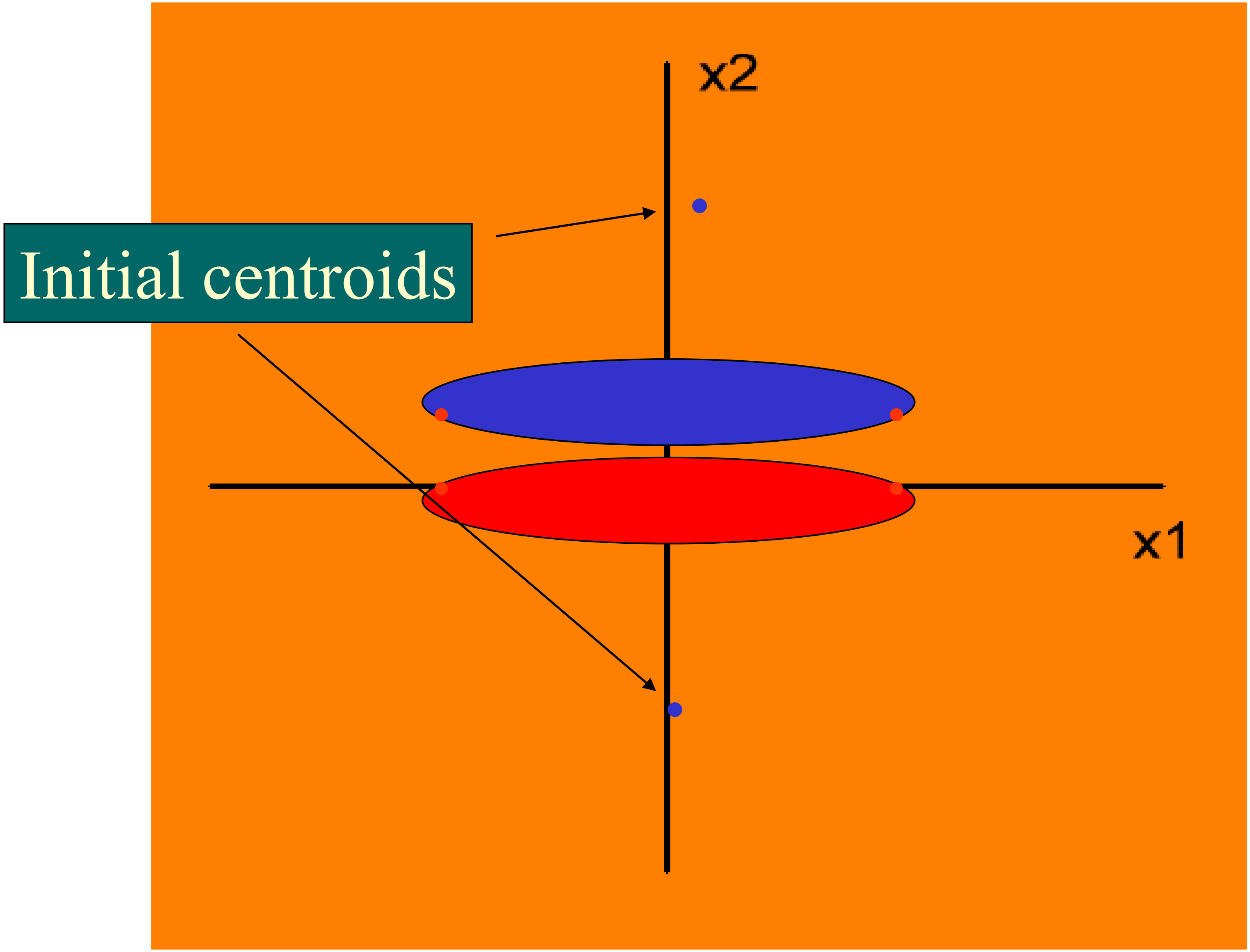
- The result depends on the initialization.
- J is not minimized
- The results are sometimes “intuitively wrong”.

N-means clustering – An example

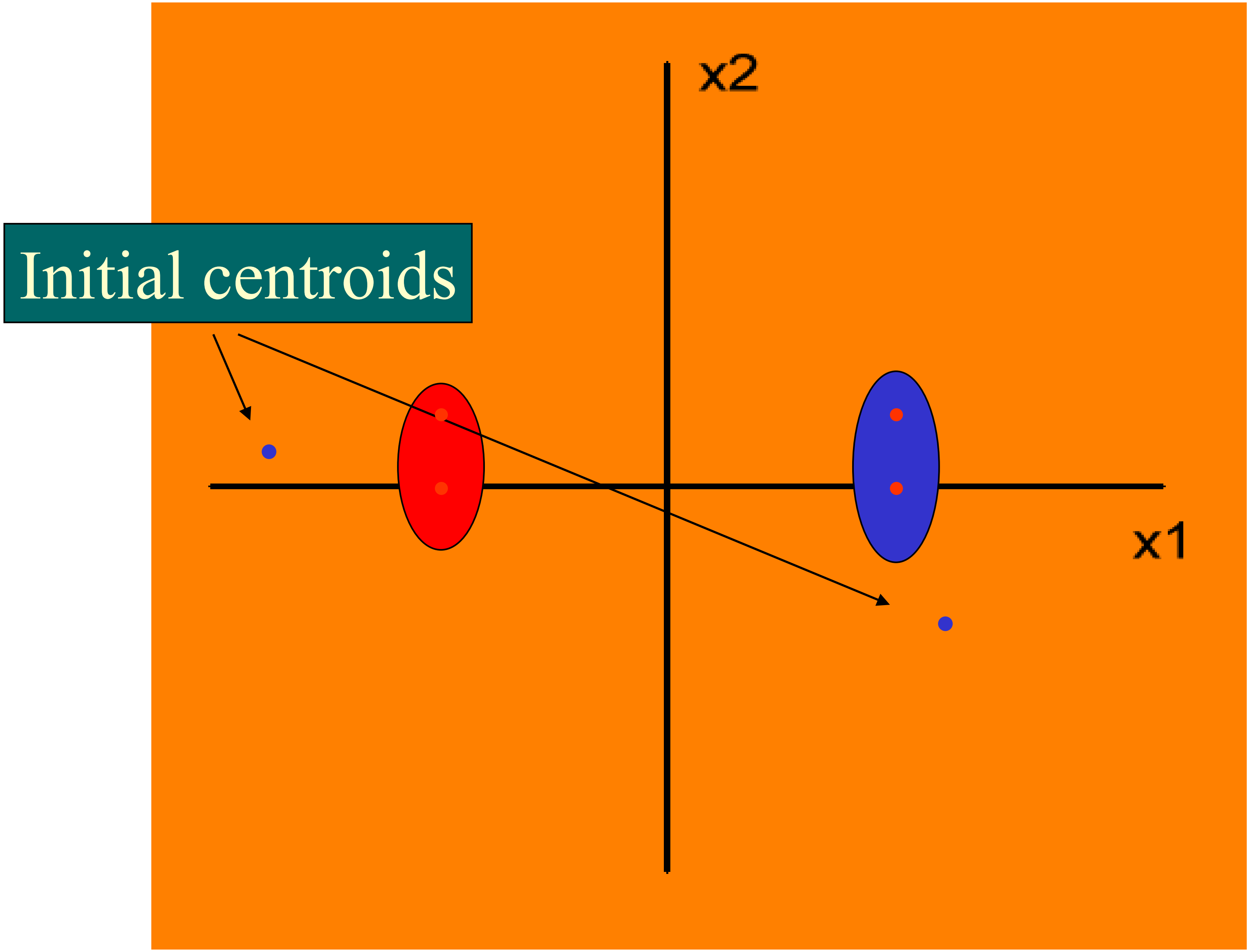
Two features, four points, two clusters ($N = 2$)

Different initializations → different clusterings

N-means clustering – An example



N-means clustering – An example



Iterative minimization of J

1. Let's have an initial clustering (by N-means)
2. For every point x do the following:

   Move x from its current cluster to another cluster, such that the decrease of J is maximized.
3. If all data points do not move, then STOP.

Iterative minimization of *J*

Drawbacks

- The algorithm is optimal in each step but in general global minimum of *J* is not reached.

ISODATA

Iterative clustering, *N* may vary.

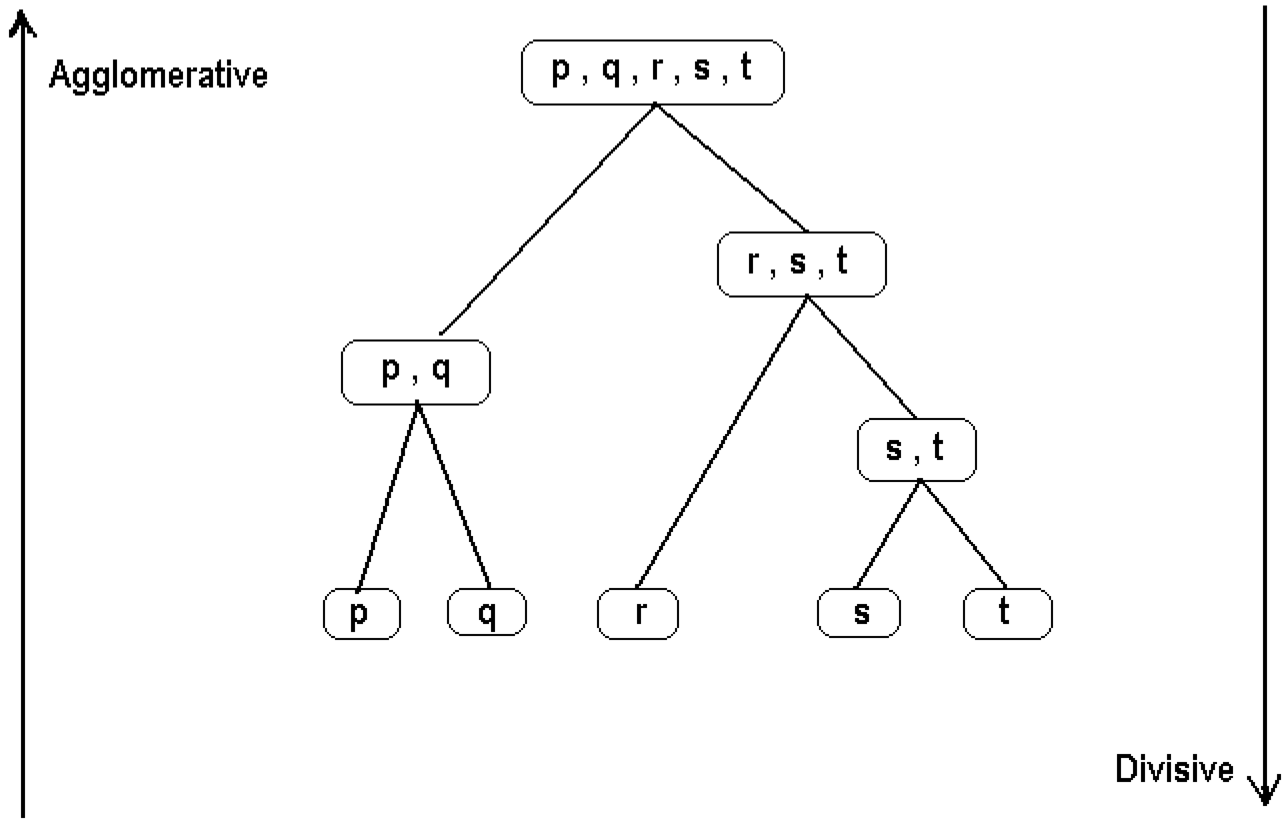
Sophisticated method, a part of many statistical software systems.

Postprocessing after each iteration

- Clusters with few elements are cancelled
- Clusters with big variance are divided
- Other merging and splitting strategies can be implemented

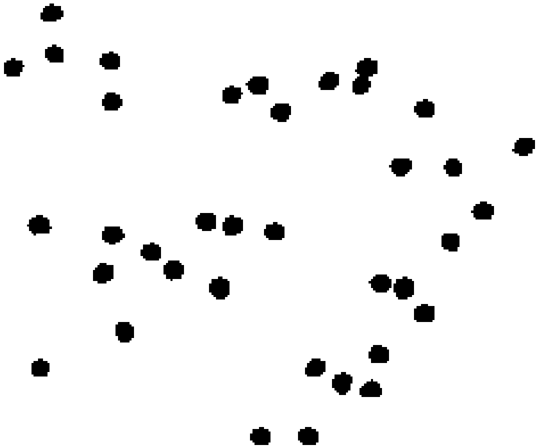
Hierarchical clustering methods

- Agglomerative clustering
- Divisive clustering



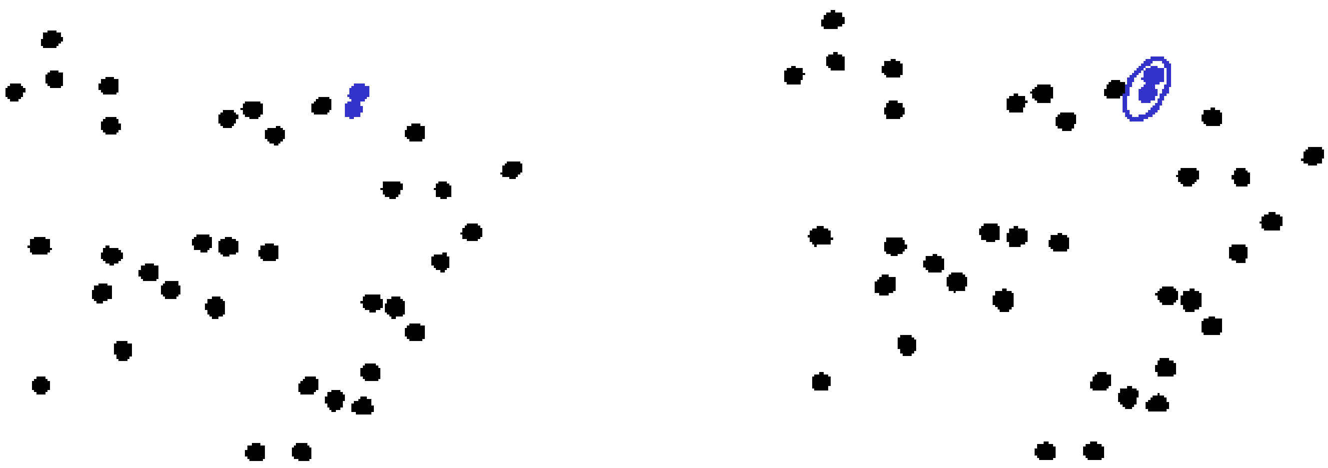
Basic agglomerative clustering

1. Each point = one cluster



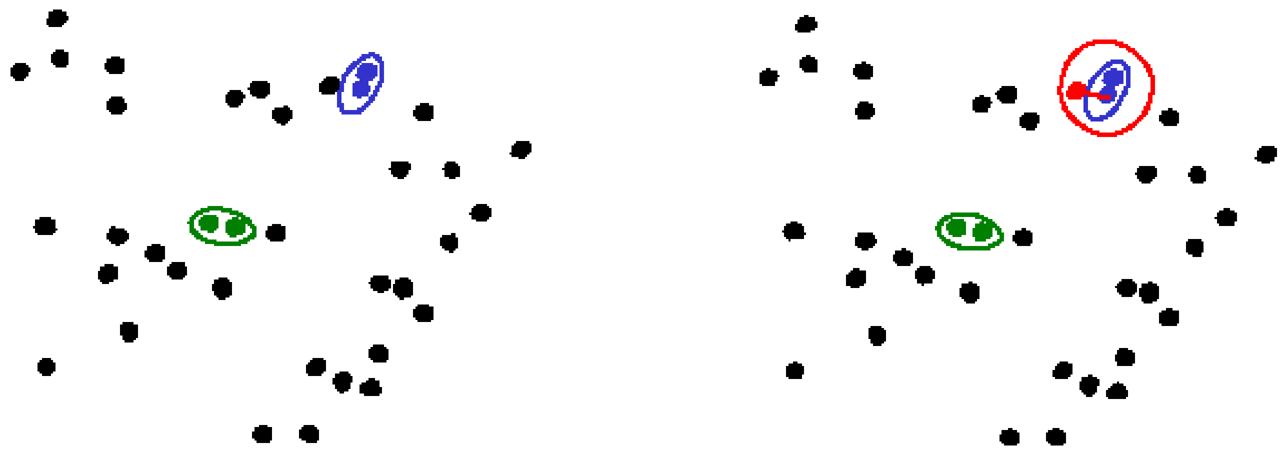
Basic agglomerative clustering

1. Each point = one cluster
2. Find two “nearest” or “most similar” clusters and merge them together



Basic agglomerative clustering

1. Each point = one cluster
2. Find two “nearest” or “most similar” clusters and merge them together
3. Repeat 2 until the stop constraint is reached



Basic agglomerative clustering

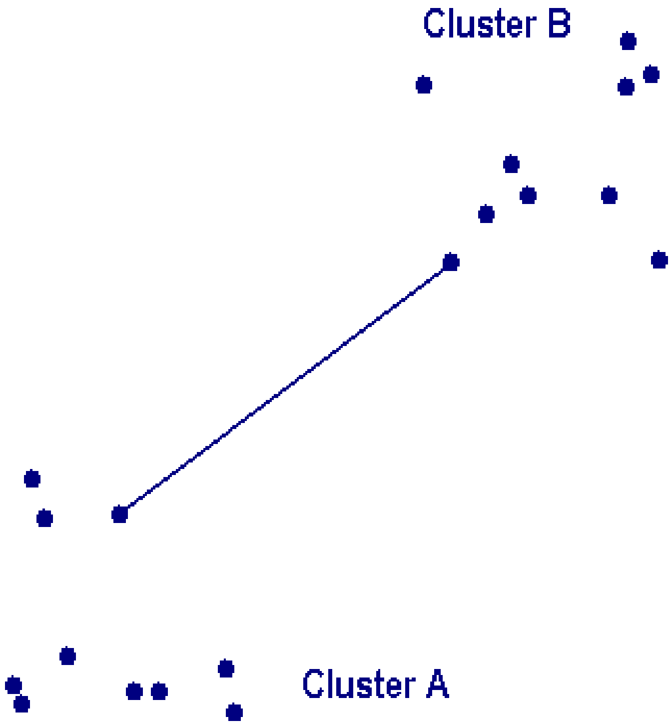
Particular implementations of this method differ from each other by

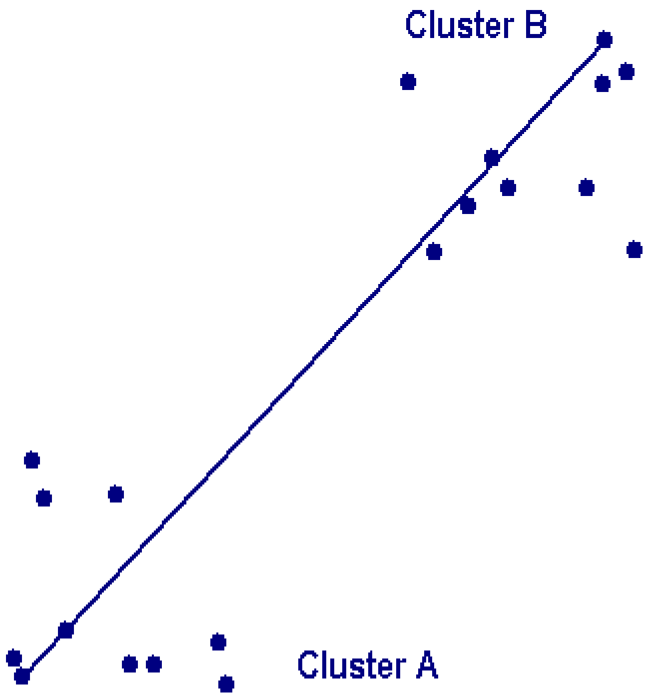
- The STOP constraints
- The distance/similarity measures used

Simple between-cluster distance measures

$$d(A,B) = d(m_1, m_2)$$

$$d(A,B) = \min d(a,b) \qquad\qquad d(A,B) = \max d(a,b)$$





Other between-cluster distance measures

$d(A,B)$ = Hausdorf distance $H(A,B)$

$$d(A,B) = J(A \cup B) - J(A,B)$$

Efficient implementation of hierarchical clustering

At each level, the distances are calculated using the distances from the previous level.

The upgrade is much faster than a complete calculation.

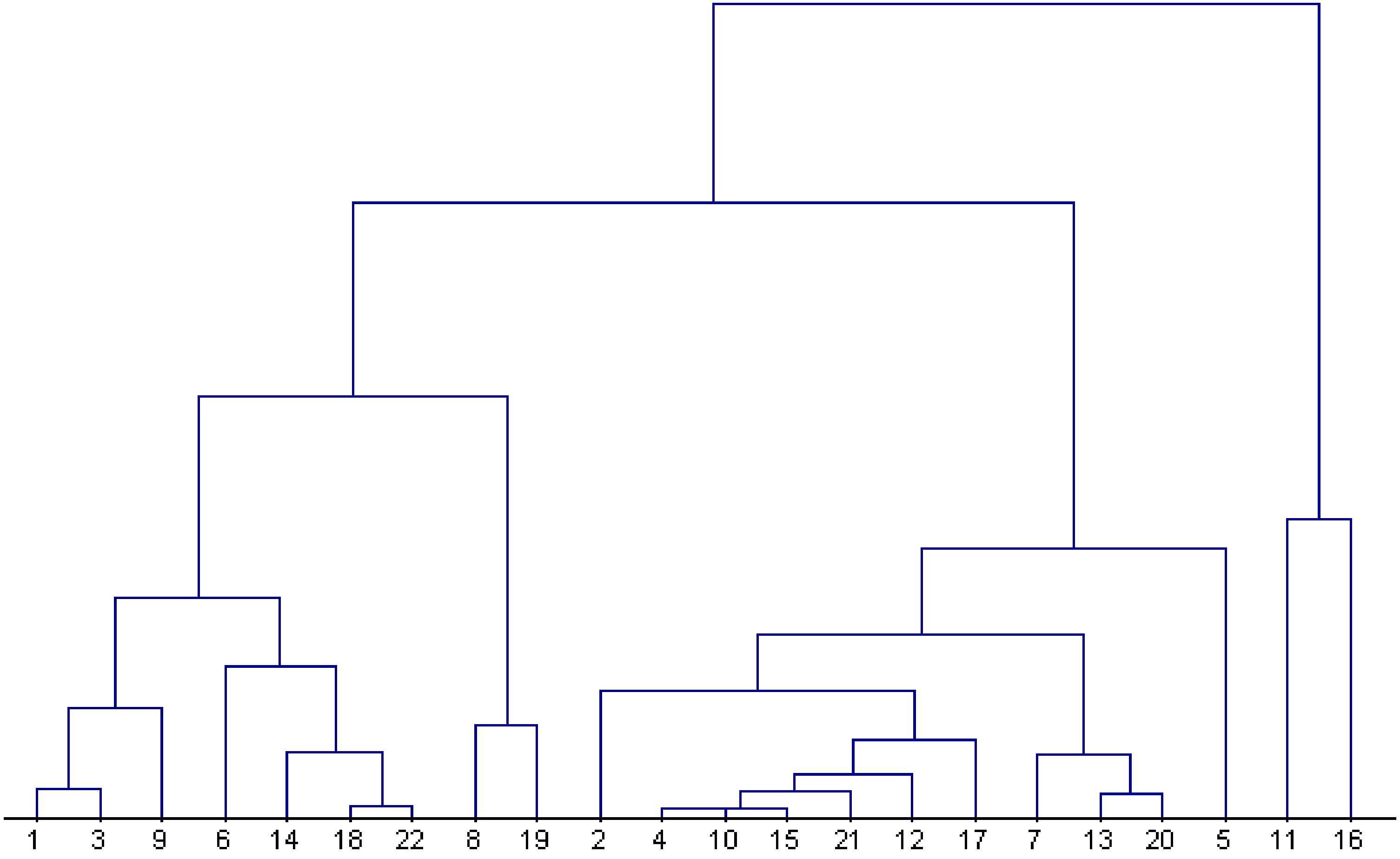
Definite agglomerative clustering

Basic algorithm – at a certain level, there may be multiple candidates of merging.

Random selection leads to ambiguities.

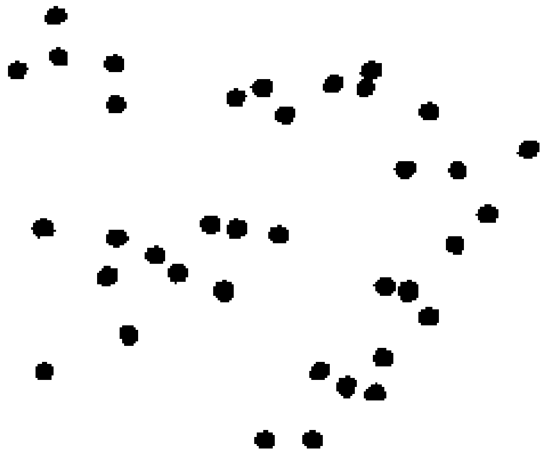
Definite algorithm – **all** such candidates are merged at that level → the number of new clusters emerging at one level may be greater than 1.

Agglomerative clustering – representation by a clustering tree (dendrogram)



Basic divisive clustering

1. All points = one cluster



Basic divisive clustering

1. All points = one cluster
2. Divide the cluster into two parts A,B such that $d(A,B)$ is maximized
3. Select a new cluster to split
4. Apply 2 to the selected cluster
5. Repeat 3-4 until the stop constraint is reached

Full search in Step 2 is very expensive – $O(2^n)$

Suboptimal Step 2 of divisive clustering

1. Find point *p* such that the mean of *d(p,x)* is maximized
2. Divide C into A U B, where B={*p*} (*p* is a seed point of a new cluster B)
3. For *x* from A calculate the mean dist *d(x,A)* and *d(x,B)*. If *d(x,A)* > *d(x,B)* move *x* into B.
4. Repeat 3 for each *x* from A.

Suboptimal Step 2 of divisive clustering

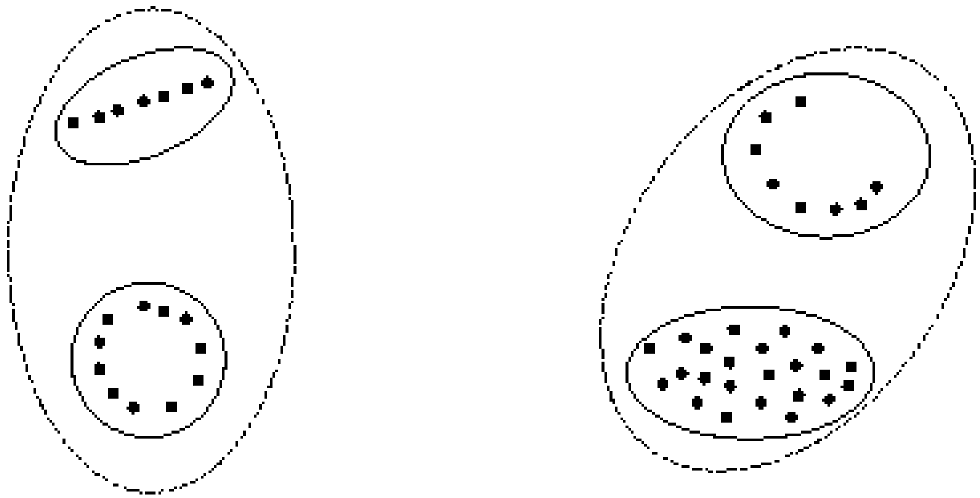
Alternatively, any iterative algorithm for N=2 can be used (N-means, J - minimization, ...)

Step 3 of divisive clustering

Selecting the next cluster to split

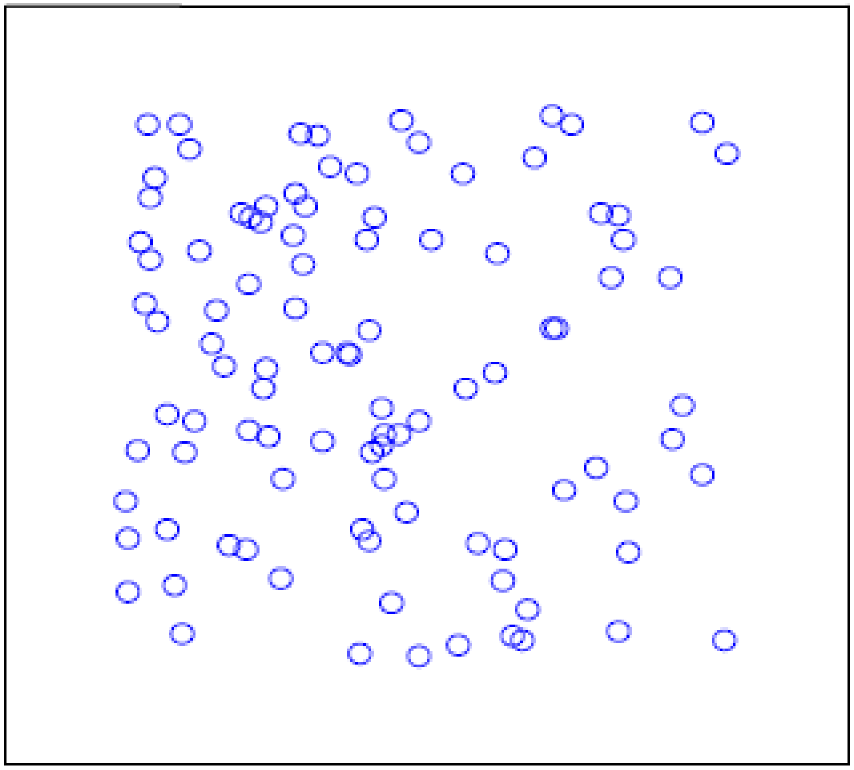
- randomly (when performing complete decomposition)
- by maximum diameter
- by maximum variance
- by maximum *J*

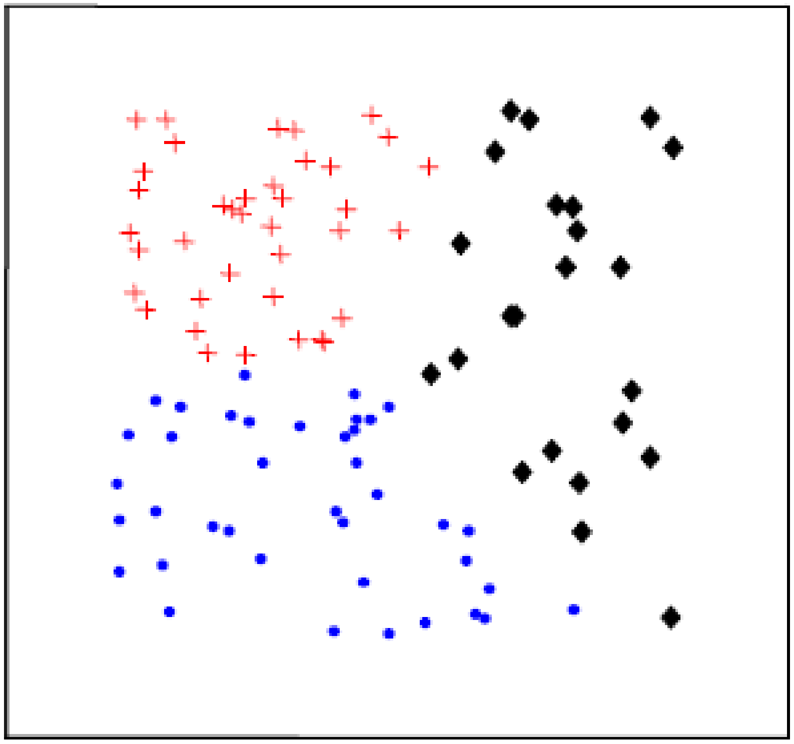
How many clusters are there?



2 or 4 ?

Clustering is a very subjective task

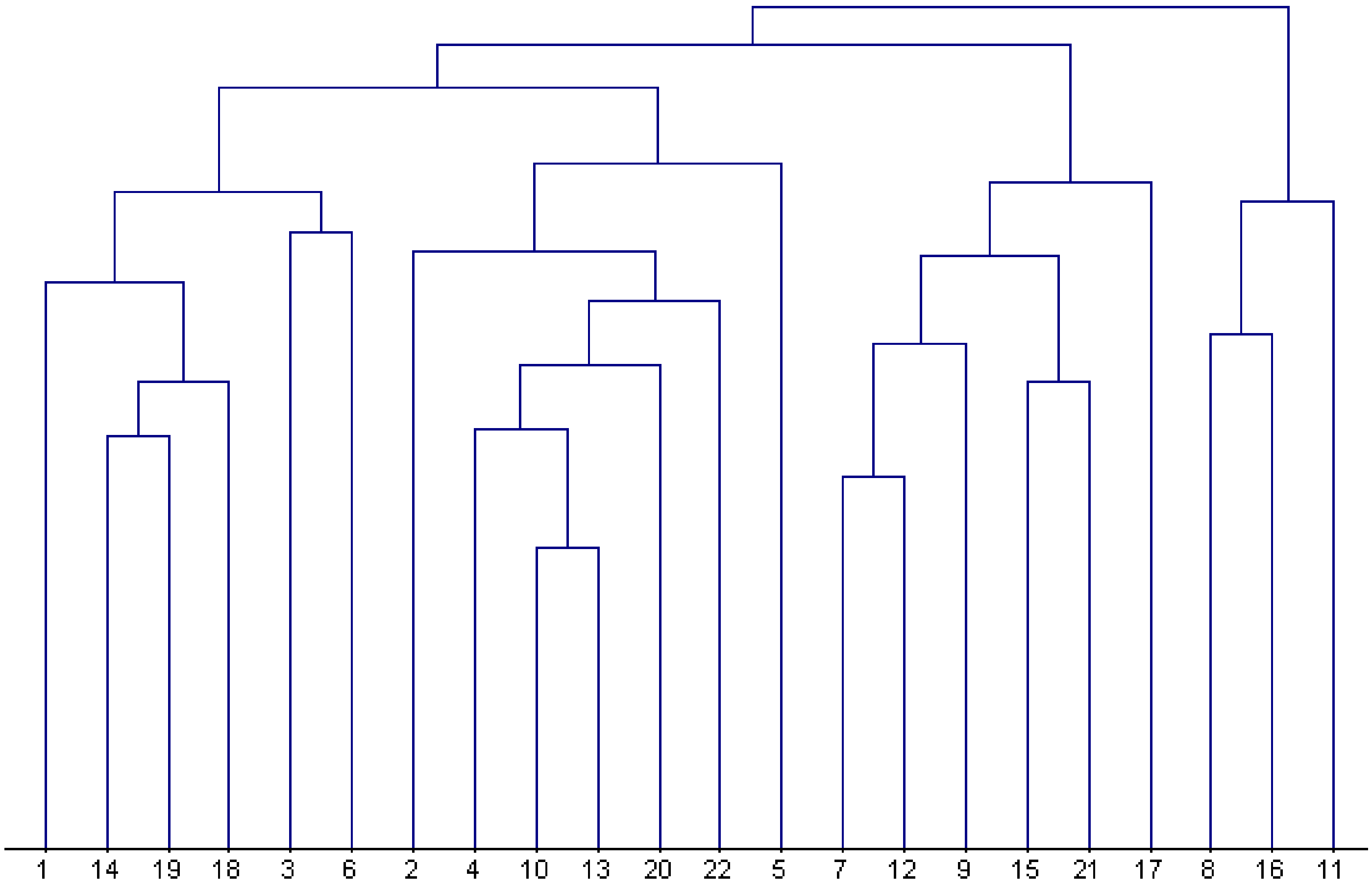




How many clusters are there?

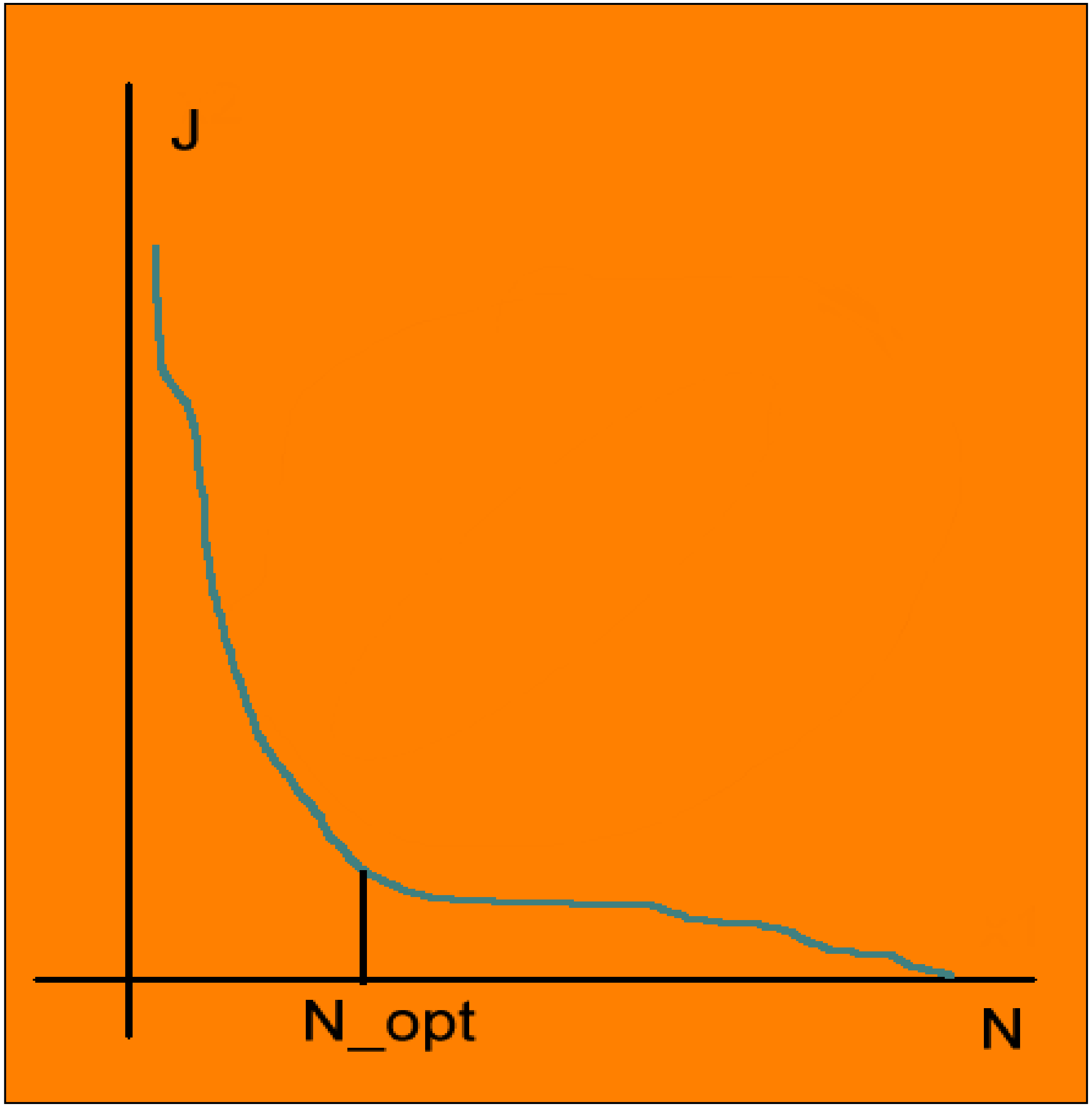
- Difficult to answer even for humans
- "Clustering tendency", "cluster validity"
- Hierarchical methods – *N* can be estimated from the complete dendrogram
- The methods minimizing a cost function – *N* can be estimated from the "knees" in *J*-*N* graph

Life time of the clusters

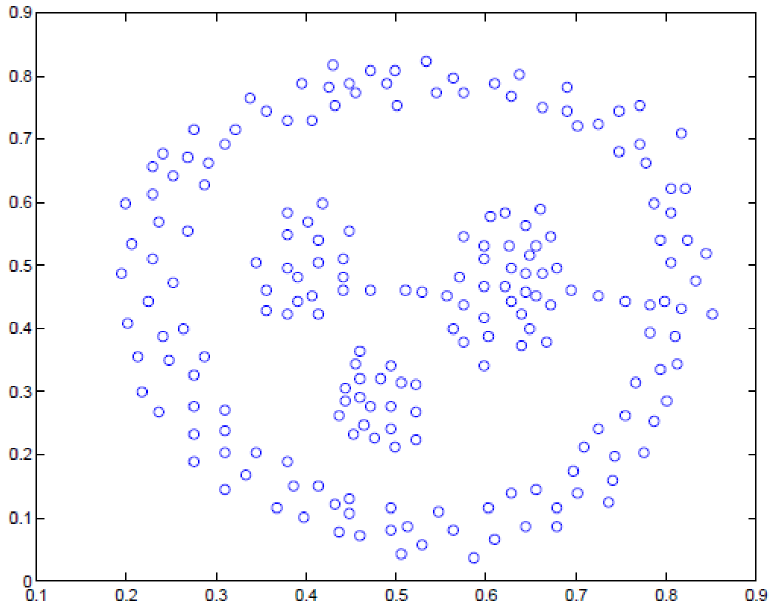


Optimal number of clusters = 4

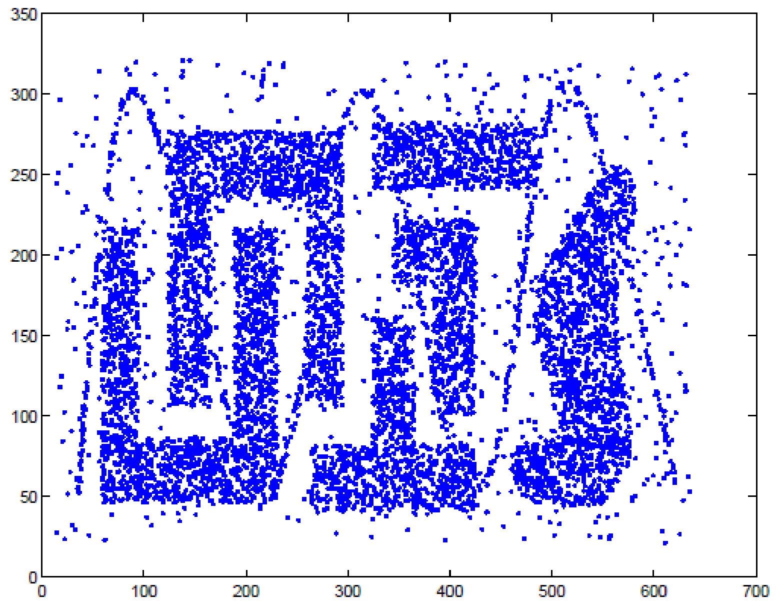
Optimal number of clusters



Hybrid clustering with the choice of N

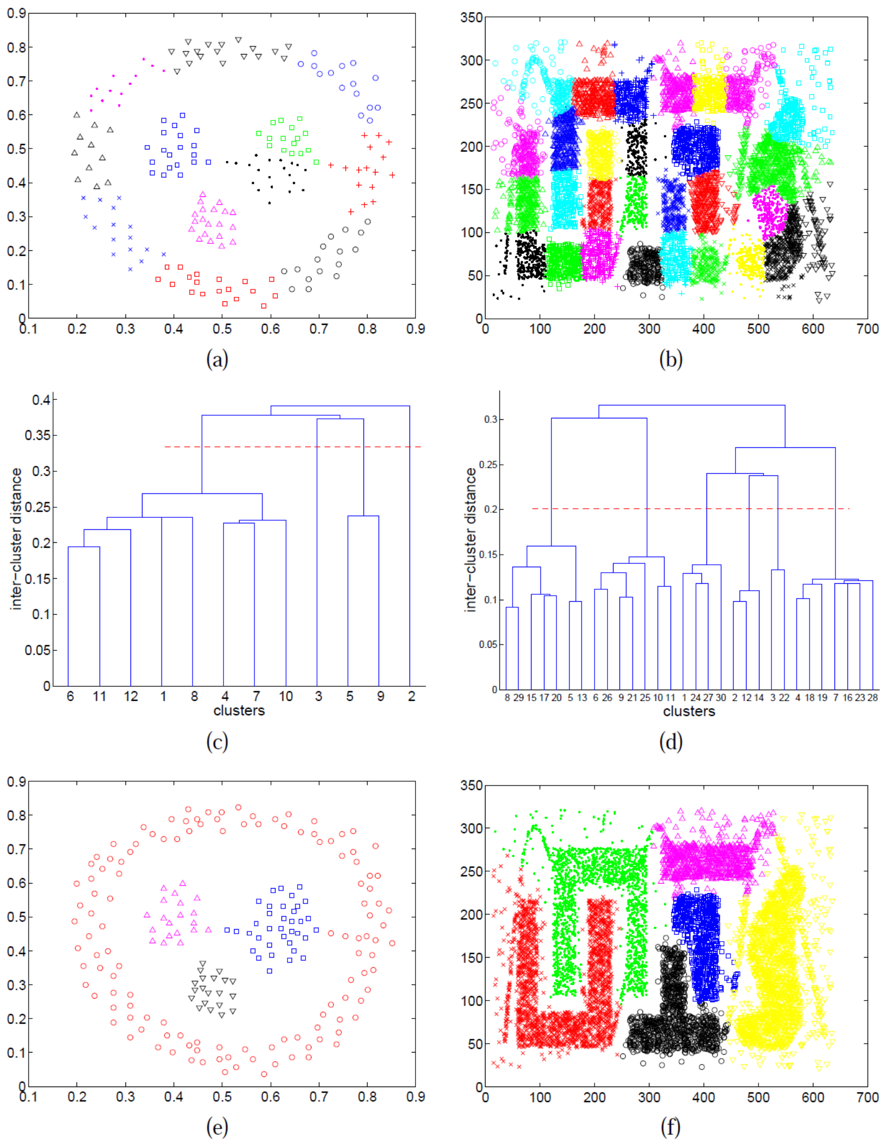


(a)



(b)

Hybrid clustering with the choice of N



Iterative

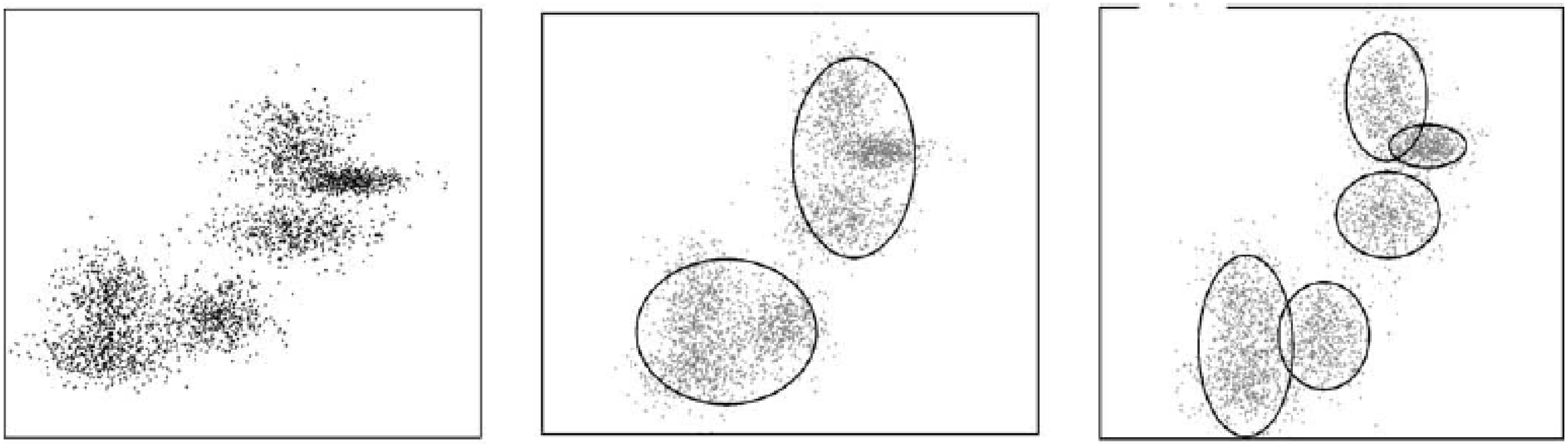
Hierarchical merging

Model-based (parametric) clustering

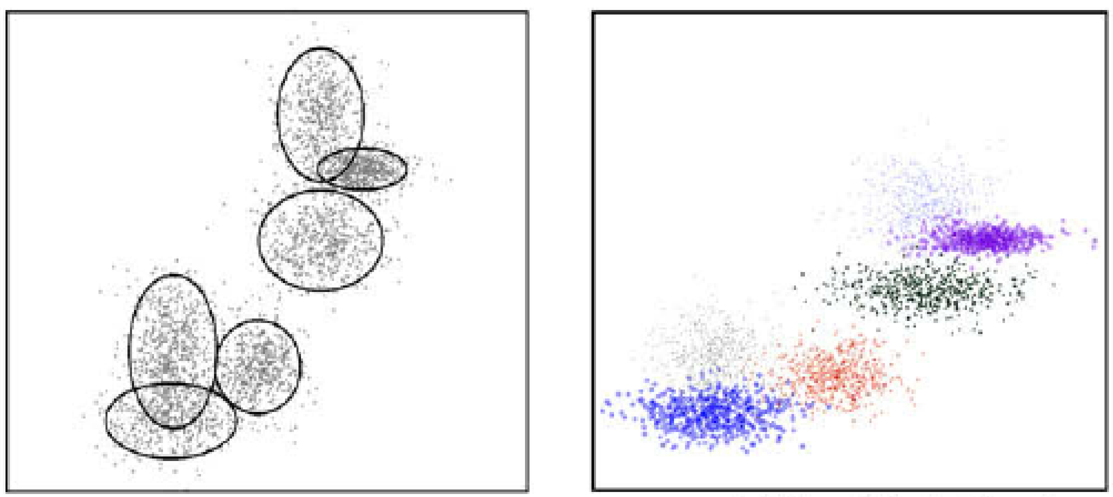
Fitting a Gaussian mixture to the data

$$f(\mathbf{x}) = \sum_{g=1}^{G} \pi_g \phi(\mathbf{x}|\mu_g, \mathbf{\Sigma}_g)$$

Problem: the number of components



(a) Input data (b) GMM (K=2) (c) GMM (K=5)

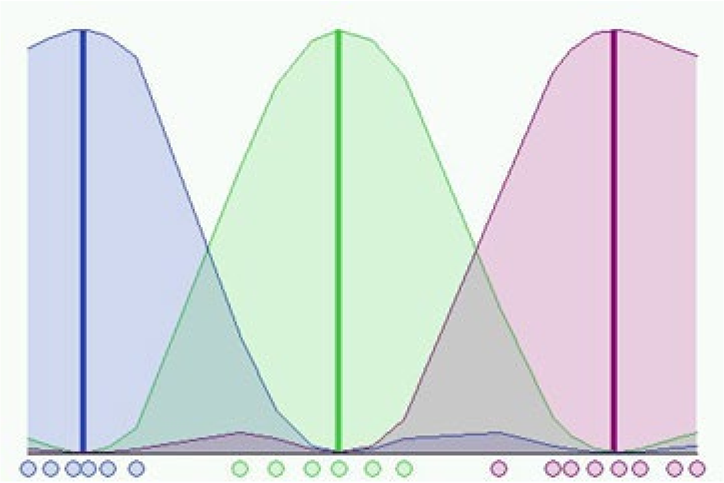


(d) GMM (K=6) (e) True labels, K = 6

Fuzzy clustering

Clusters = Fuzzy sets (Set, Mem. f)

Fuzzy C-means



Other clustering criteria

Scatter matrices

- between cluster matrix

$$B = \sum_{i=1}^{N} n_i(\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^t$$

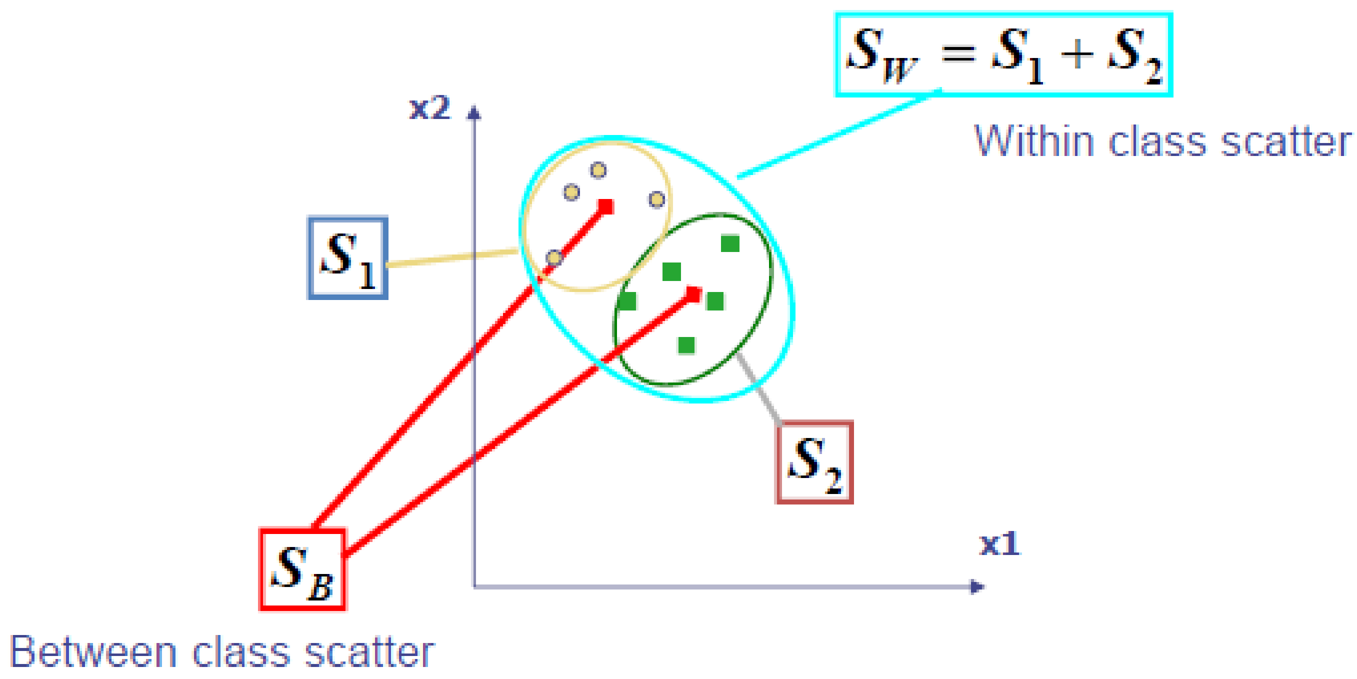
- within cluster matrix

$$W = \sum_{i=1}^{N} W_i$$

$$W_i = \sum_{\mathbf{x} \in C_i} (\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^t$$

- total scatter matrix

$$T = \sum_{\mathbf{x}} (\mathbf{x} - \mathbf{m})(\mathbf{x} - \mathbf{m})^t$$



$S_W = S_1 + S_2$
Within class scatter
x2
S_1
S_2
x1
S_B
Between class scatter

Other clustering criteria

min $\mathrm{tr}(W) = \sum_{i=1}^{N} \mathrm{tr}(W_i) = \sum_{i=1}^{N} \sum_{\mathbf{x} \in C_i} \|\mathbf{x} - \mathbf{m}_i\|^2 = J$

min $\det(W)$

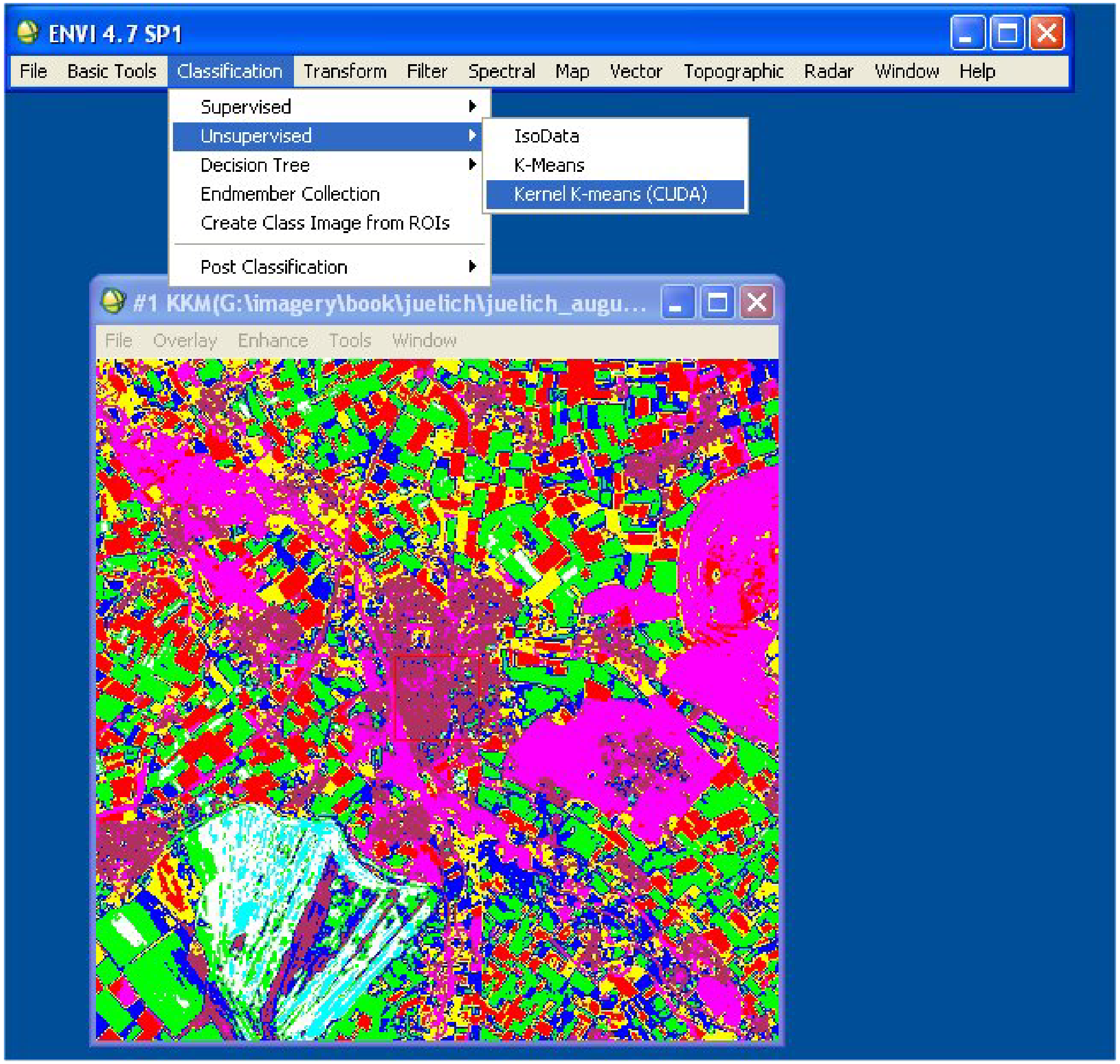
$T = W + B$

max $\mathrm{tr}(W^{-1}B)$

Applications of clustering in image proc.

- Segmentation – clustering in color space
- Preliminary classification of multispectral images
- Clustering in parametric space – RANSAC, image registration and matching

Numerous applications are outside image processing area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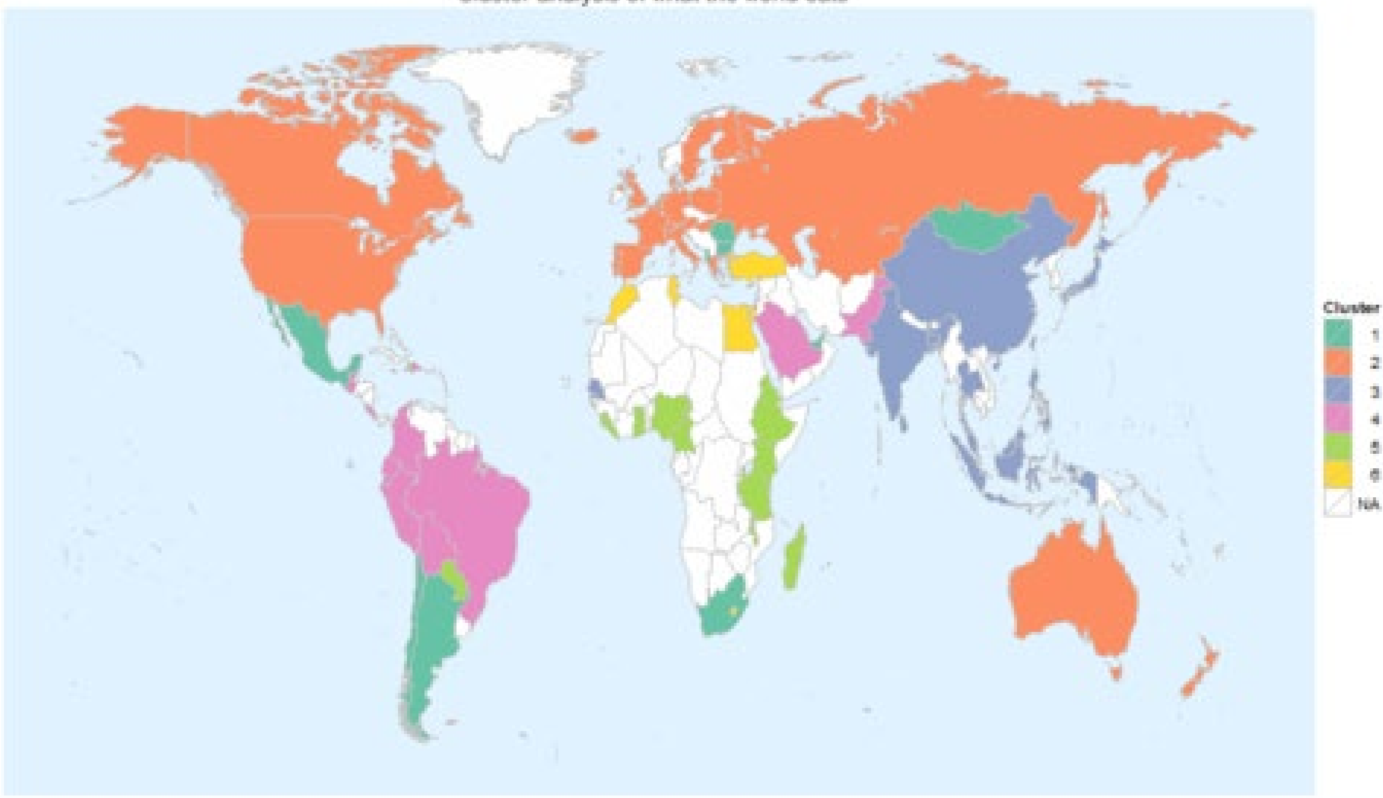
Cluster analysis of what the world eats



Thank you !

Any questions ?