Pattern Analysis and Machine Intelligence

Lecture Notes on Clustering (II)
2010-2011

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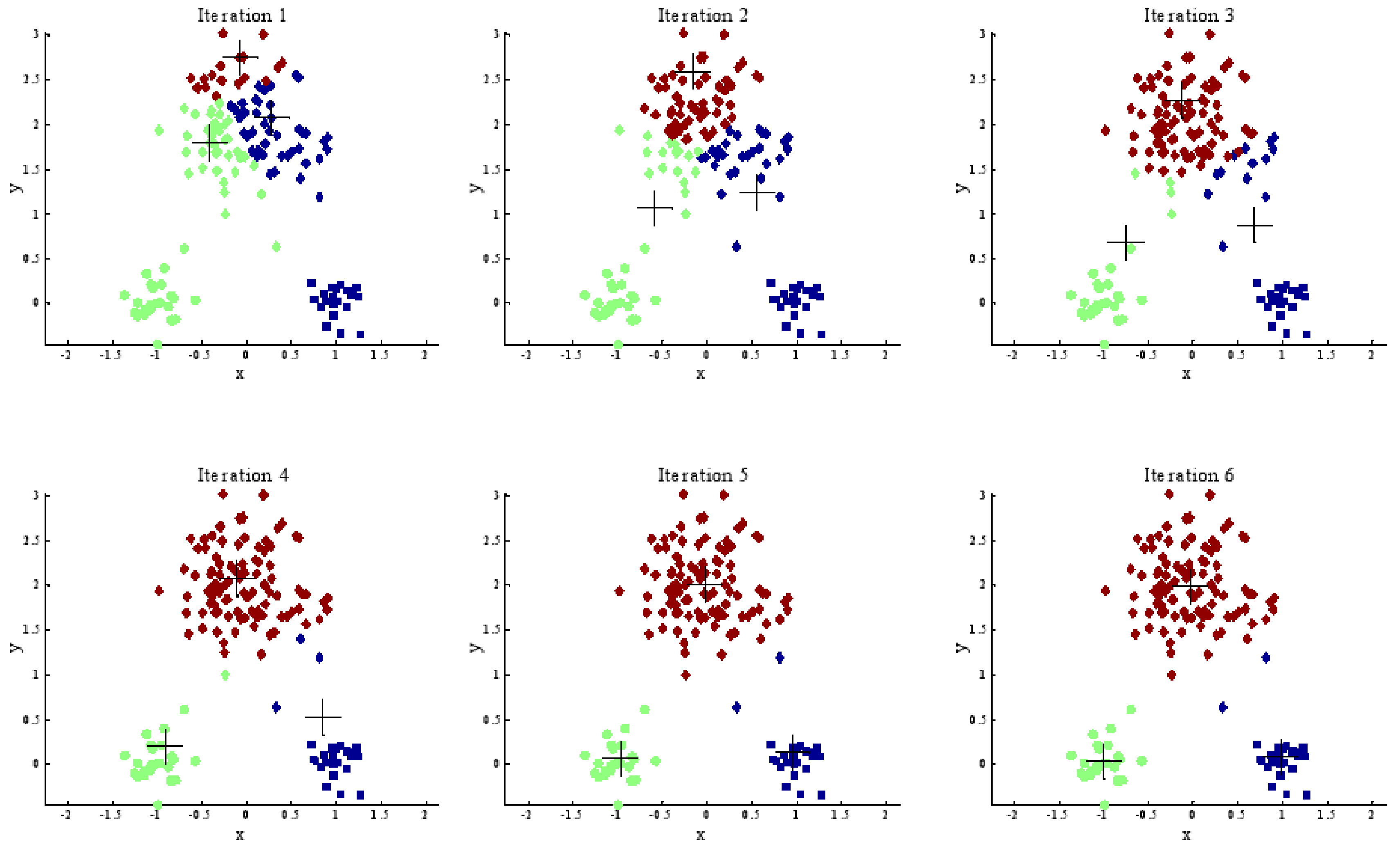
Course Schedule [*Tentative*]

Date	Topic
13/04/2011	Clustering I: Introduction, K-means
20/04/2011	Clustering II: K-M alternatives, Hierarchical, SOM
27/04/2011	Clustering III
04/05/2011	Clustering IV

K-Means limits

Importance of choosing initial centroids



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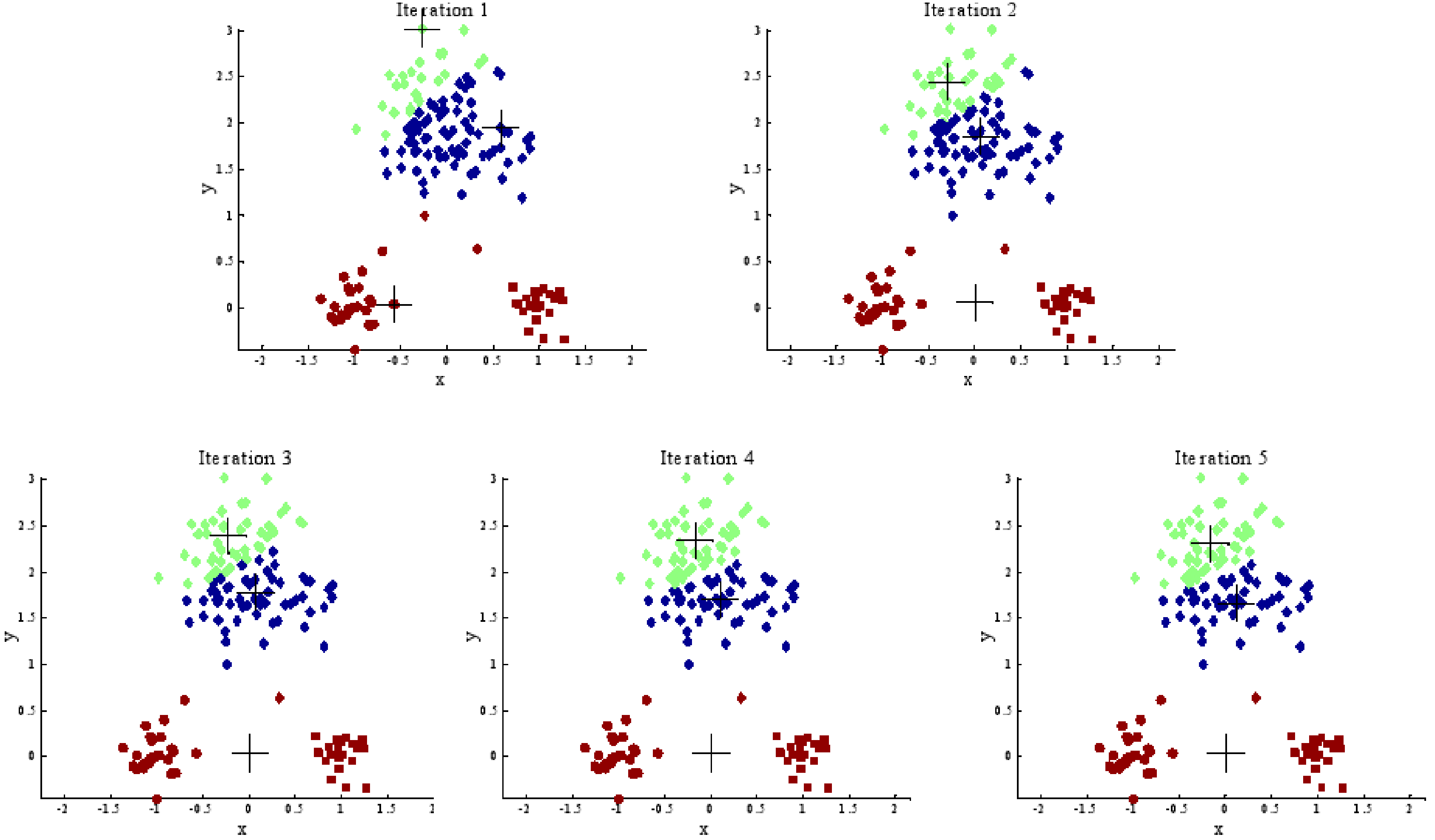
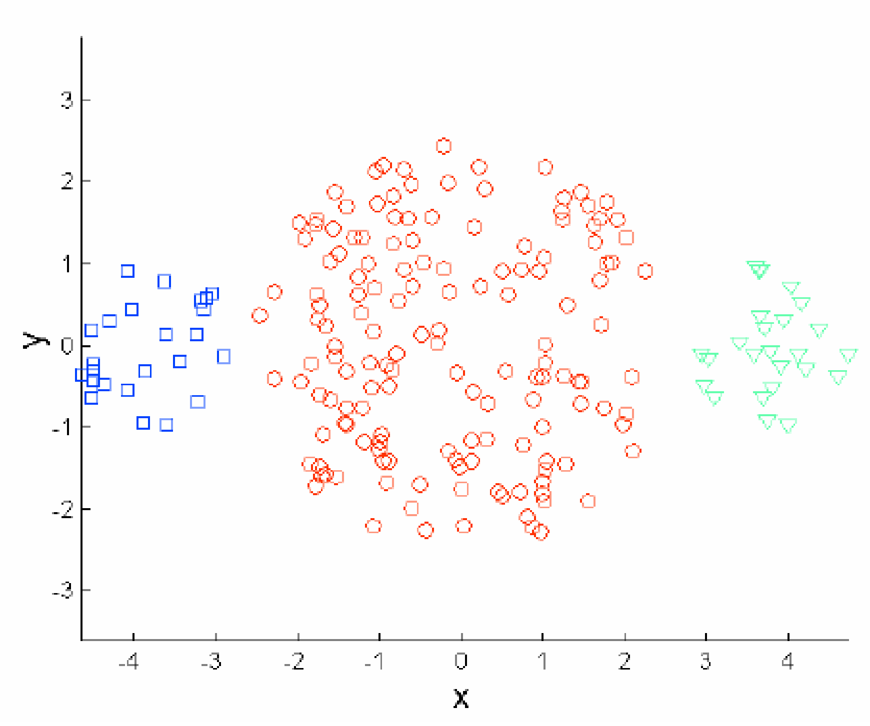
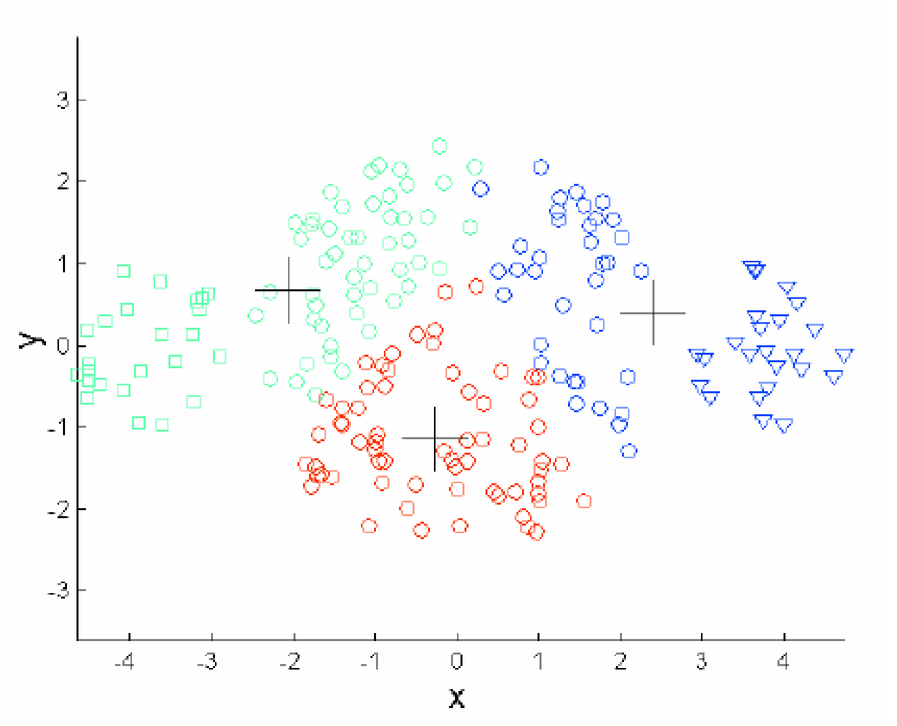


K-Means limits

Differing sizes

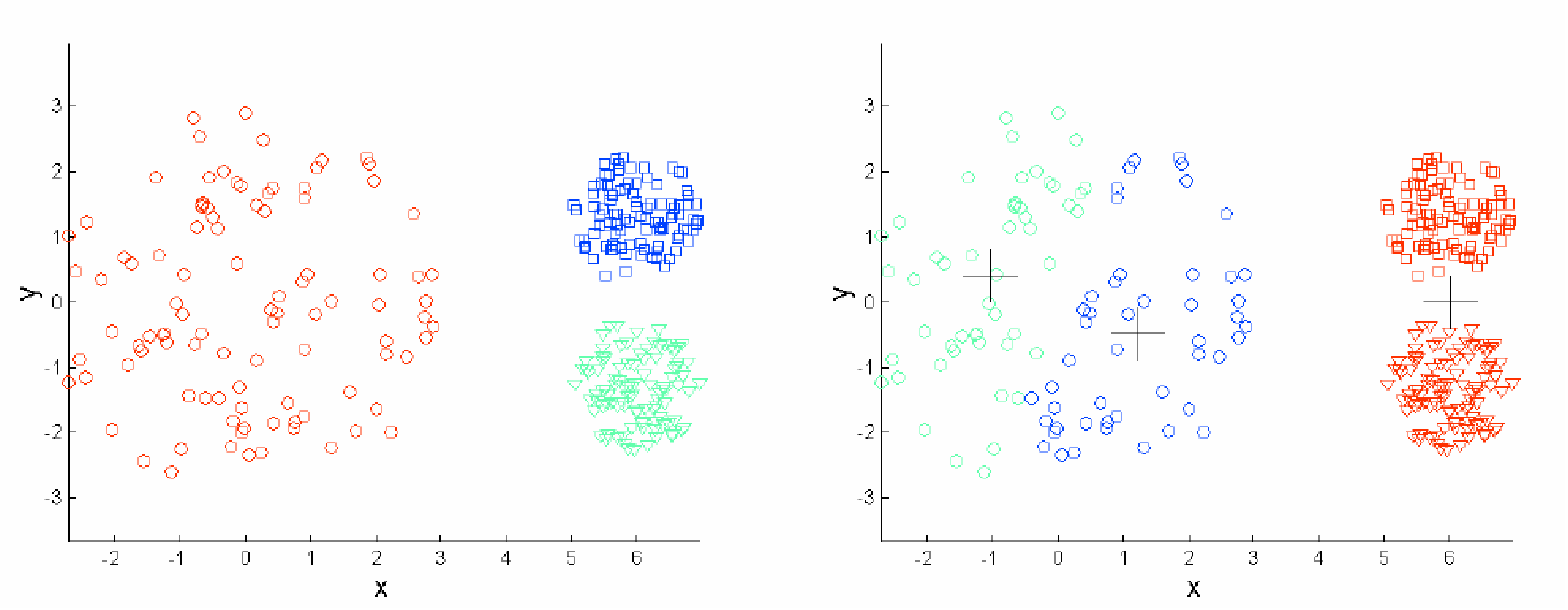




Original Points **K-means Clusters**

K-Means limits

Differing density



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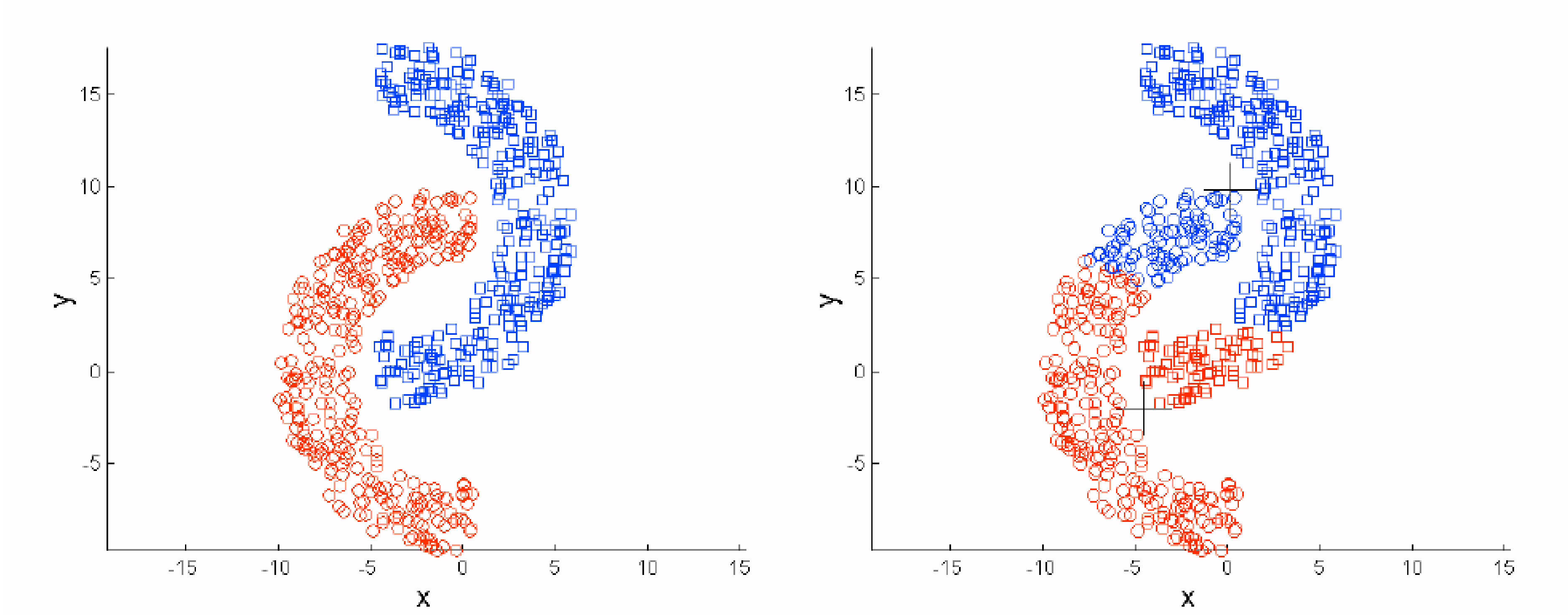
Non-globular shapes



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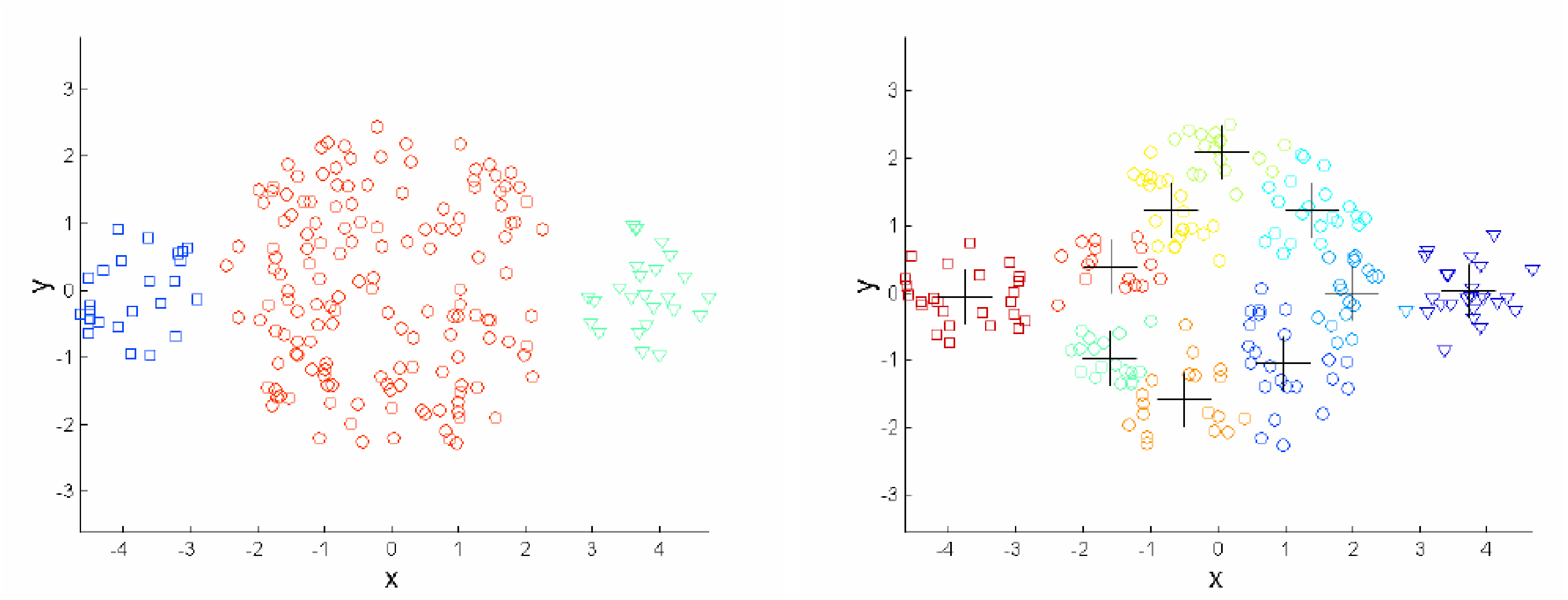
K-Means: higher K

What if we tried to increase K to solve K-Means problems?



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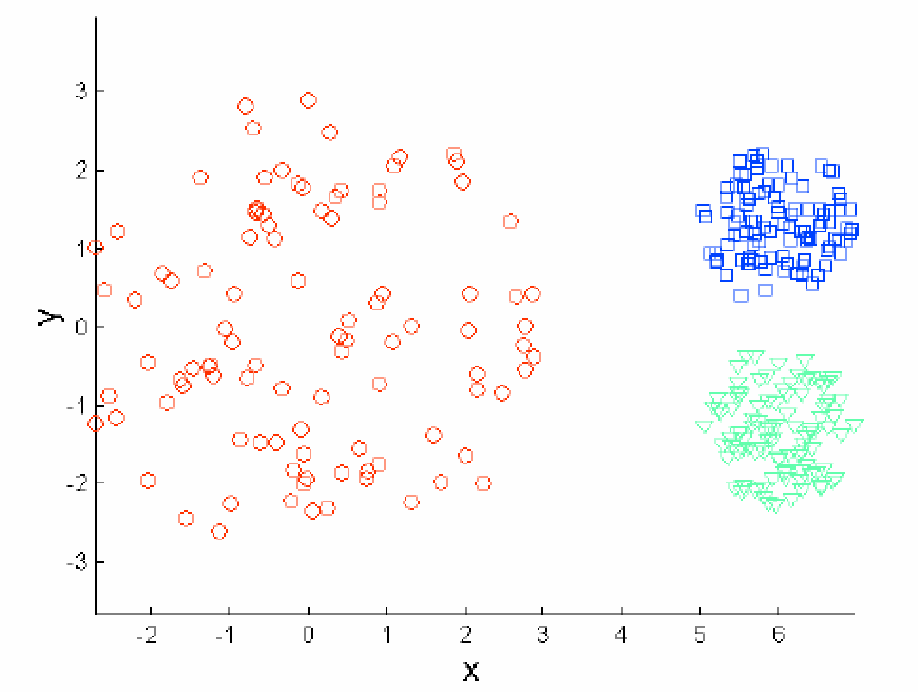

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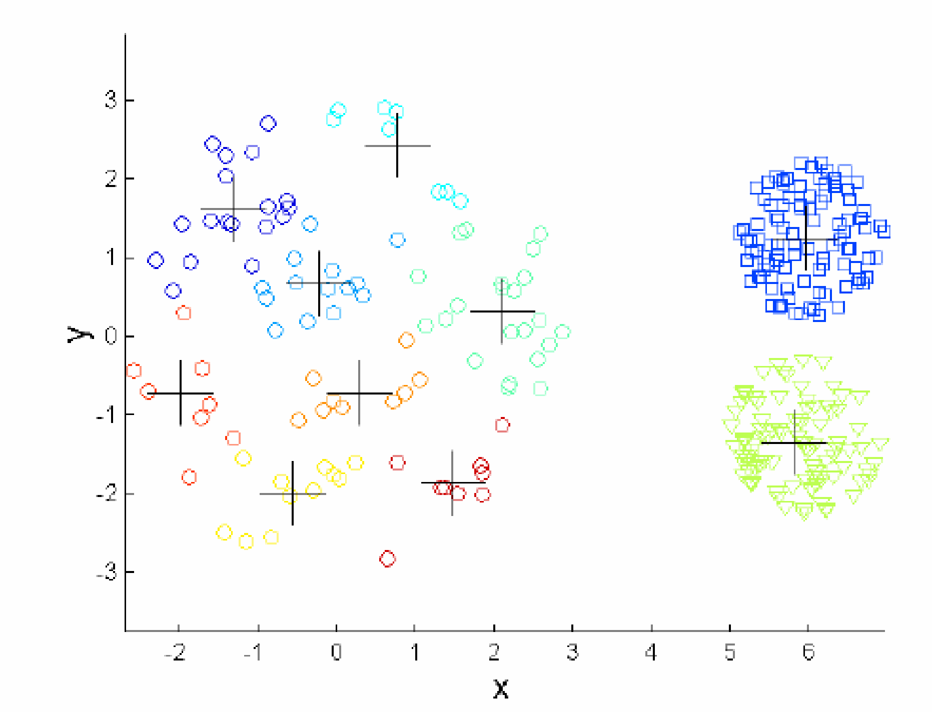

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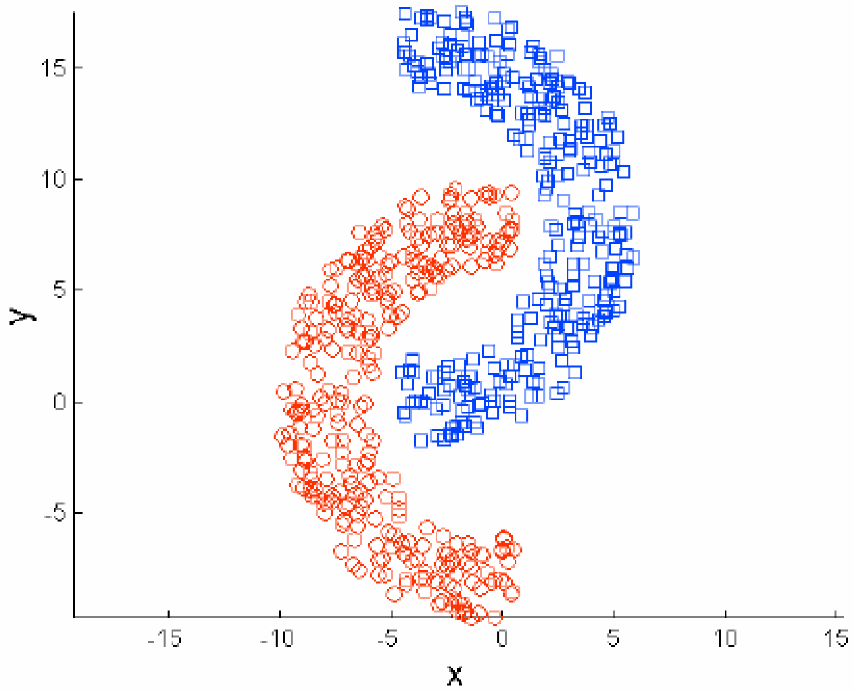

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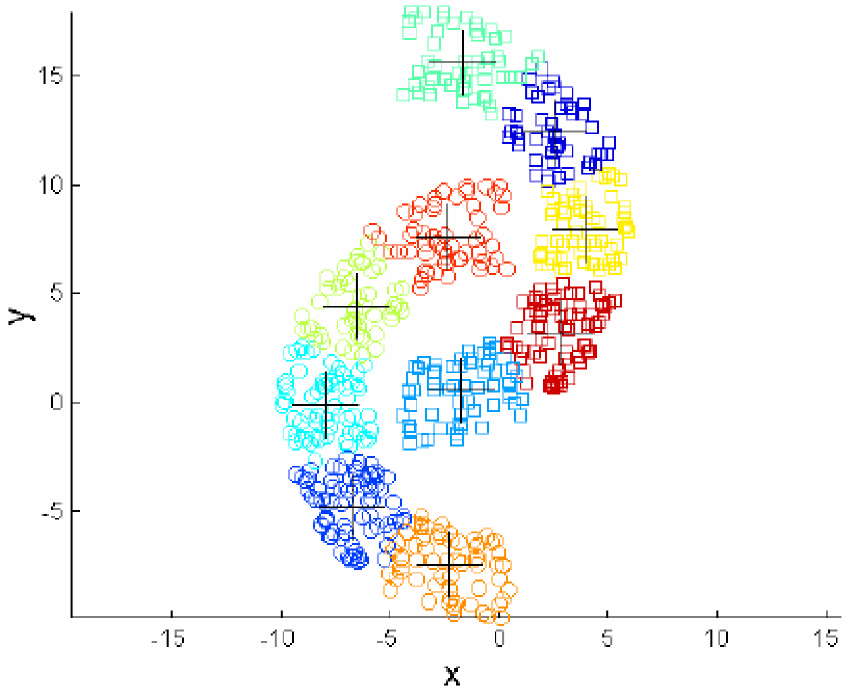


K-means Clusters

K-Medoids

- K-Means algorithm is too sensitive to outliers
  - An object with an extremely large value may substantially distort the distribution of the data
- **Medoid**: the most centrally located point in a cluster, as a representative point of the cluster
- Note: while a medoid is always a point inside a cluster too, a centroid could be not part of the cluster.
- Instead of *means*, use *medians* of each cluster
  - Mean of 1, 3, 5, 7, 9 is 5
  - Mean of 1, 3, 5, 7, 1009 is 205
  - Median of 1, 3, 5, 7, 1009 is 5

PAM

PAM means **P**artitioning **A**round **M**edoids. The algorithm follows:

1. Given k
2. Randomly pick k instances as initial medoids
3. Assign each data point to the nearest medoid x
4. Calculate the objective function
   - the sum of dissimilarities of all points to their nearest medoids. (squared-error criterion)
5. For each non-medoid point y
   - swap x and y and calculate the objective function
6. Select the configuration with the lowest cost
7. Repeat (3-6) until no change

PAM

- Pam is more robust than k-means in the presence of noise and outliers
  - A medoid is less influenced by outliers or other extreme values than a mean (can you tell why?)
- Pam works well for small data sets but does not scale well for large data sets
  - $O(k(n-k)^2)$ for each change where n is # of data objects, k is # of clusters
- NOTE: not having to calculate a *mean*, we do not need actual *positions* of points but just their *distances*!

Fuzzy C-Means

Fuzzy C-Means (FCM, developed by Dunn in 1973 and improved by Bezdek in 1981) is a method of clustering which allows one piece of data to belong to two or more clusters.

- frequently used in pattern recognition
- based on minimization of the following objective function:

$$J_m = \sum_{i=1}^{N} \sum_{j=1}^{C} u_{ij}^m \|x_i - c_j\|^2, 1 \leq m < \infty$$

where:

m is any real number greater than 1 (*fuzziness coefficient*),

u_{ij} is the degree of membership of x_i in the cluster j,

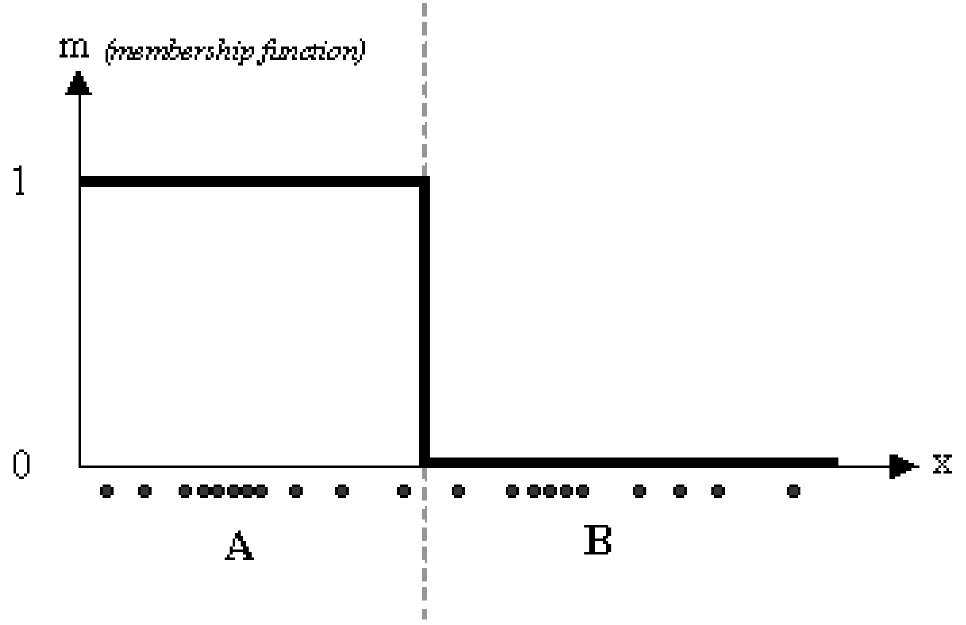
x_i is the i-th of d-dimensional measured data,

c_j is the d-dimension center of the cluster,

$\|\cdot\|$ is any norm expressing the similarity between measured data and the center.

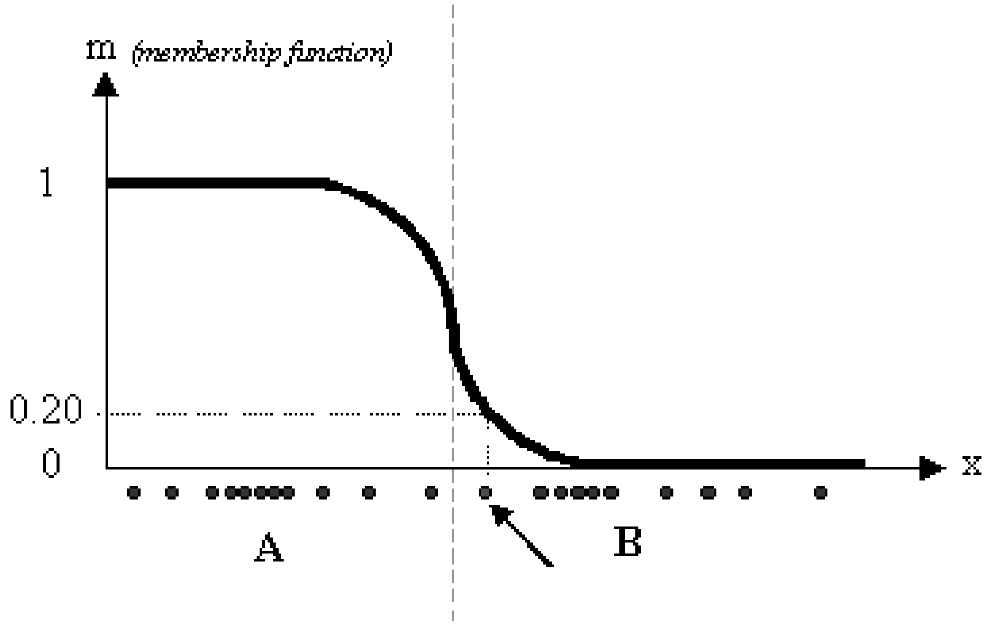
K-Means vs. FCM

- With K-Means, a datum either belongs to centroid A or to centroid B



K-Means vs. FCM

- With FCM, the same datum does not belong exclusively to one cluster, but it may belong to several clusters with different values of the membership coefficient



Data representation

$$(KM)U_{N\times C} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ \dots & \dots \\ 0 & 1 \end{bmatrix}$$

$$(FCM)U_{N\times C} = \begin{bmatrix} 0.8 & 0.2 \\ 0.3 & 0.7 \\ 0.6 & 0.4 \\ \dots & \dots \\ 0.9 & 0.1 \end{bmatrix}$$

FCM Algorithm

The algorithm is composed of the following steps:

1. Initialize $U = [u_{ij}]$ matrix, $U^{(0)}$

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$$c_j = \frac{\sum_{i=1}^{N} u_{ij}^m \cdot x_i}{\sum_{i=1}^{N} u_{ij}^m}$$

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3. Update $U^{(t)}$, $U^{(t+1)}$:

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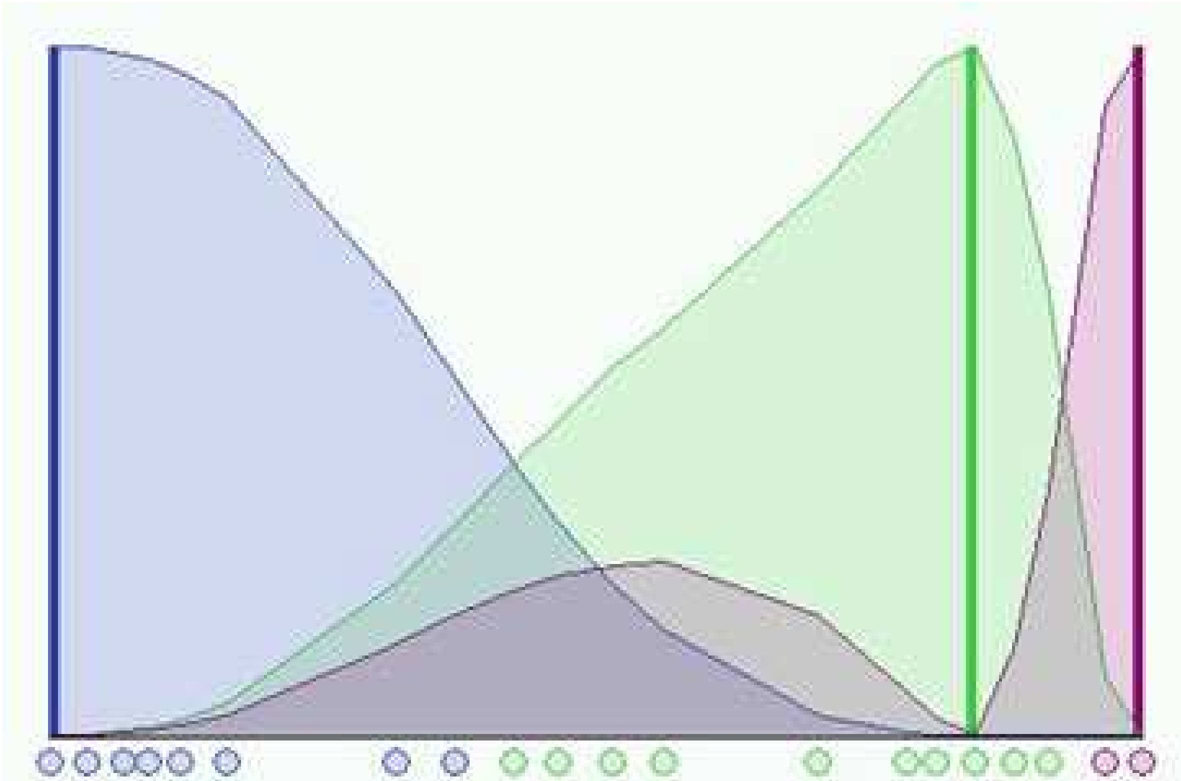
4. If $\|U^{(k+1)} - U^{(k)}\| < \varepsilon$ then STOP; otherwise return to step 2.

An Example



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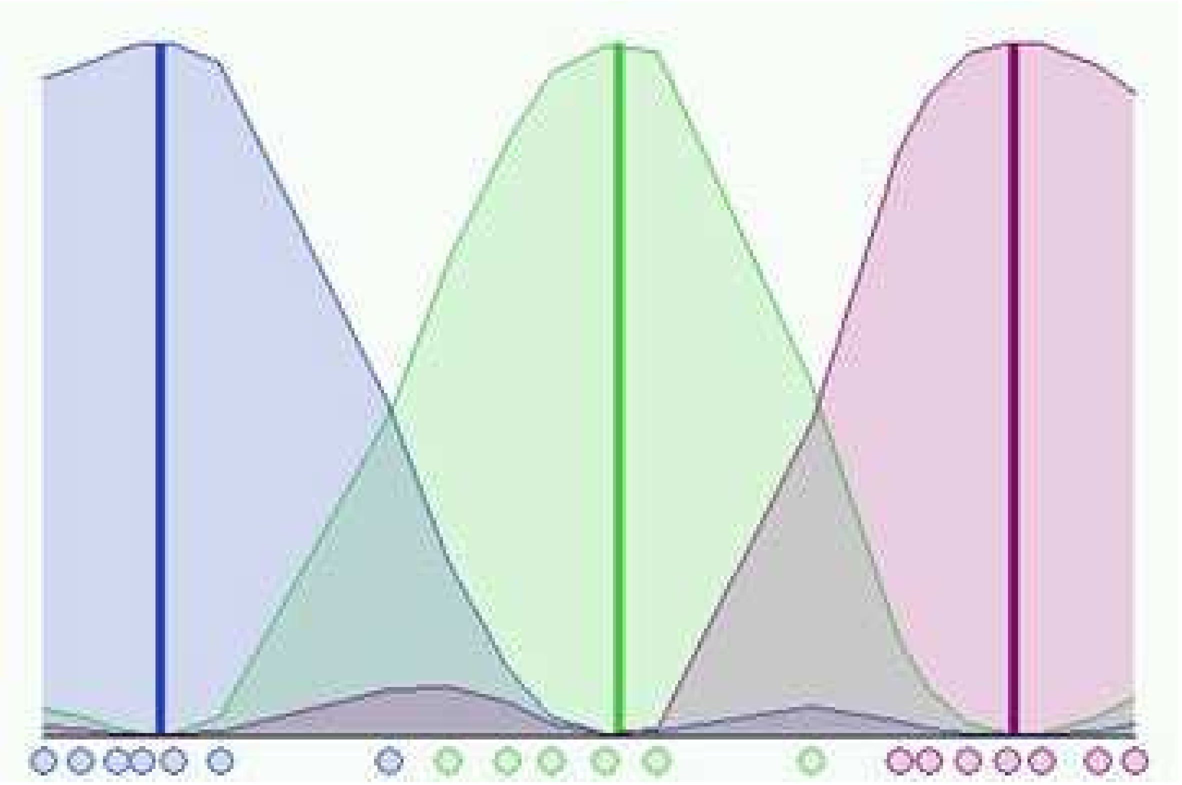

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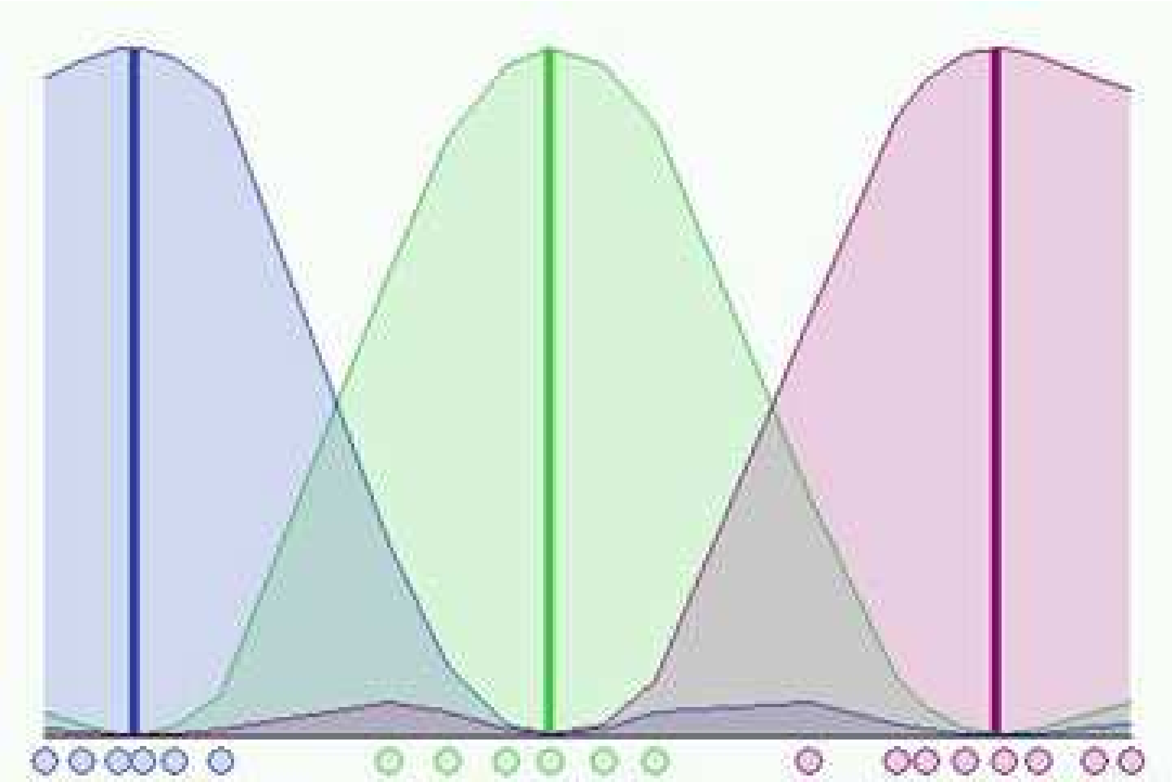


FCM Demo

Time for a demo!

Hierarchical Clustering

- Top-down vs Bottom-up
- Top-down (or *divisive*):
  - Start with one universal cluster
  - Split it into two clusters
  - Proceed recursively on each subset
- Bottom-up (or *agglomerative*):
  - Start with single-instance clusters ("every item is a cluster")
  - At each step, join the two closest clusters
  - (design decision: distance between clusters)

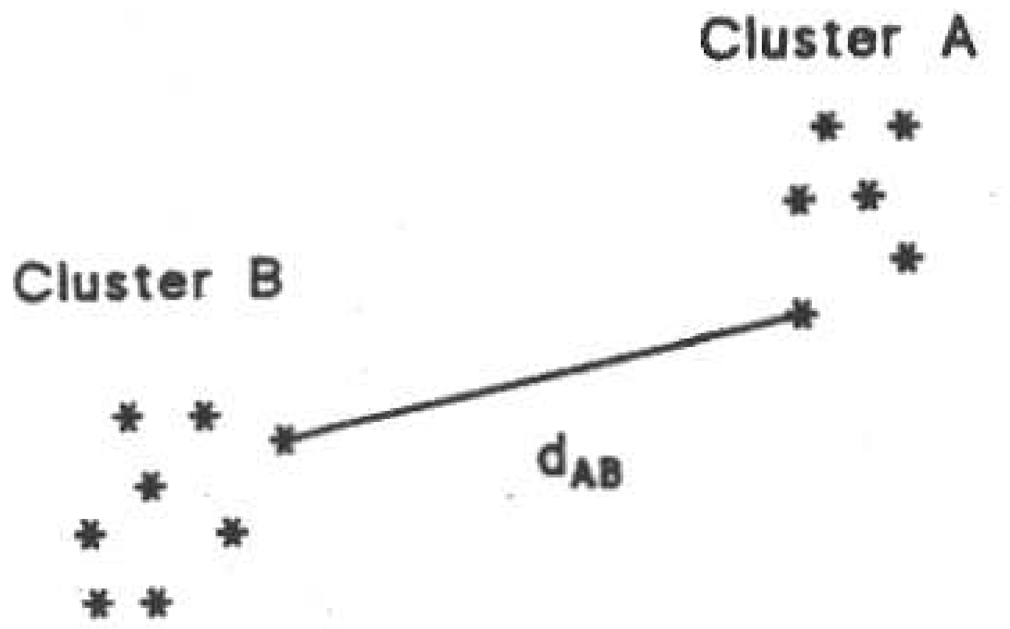
Agglomerative Hierarchical Clustering

Given a set of N items to be clustered, and an N*N distance (or dissimilarity) matrix, the basic process of agglomerative hierarchical clustering is the following:

1. Start by assigning each item to a cluster. Let the dissimilarities between the clusters be the same as the dissimilarities between the items they contain.
2. Find the closest (most similar) pair of clusters and merge them into a single cluster. Now, you have one cluster less.
3. Compute dissimilarities between the new cluster and each of the old ones.
4. Repeat Steps 2 and 3 until all items are clustered into a single cluster of size N.

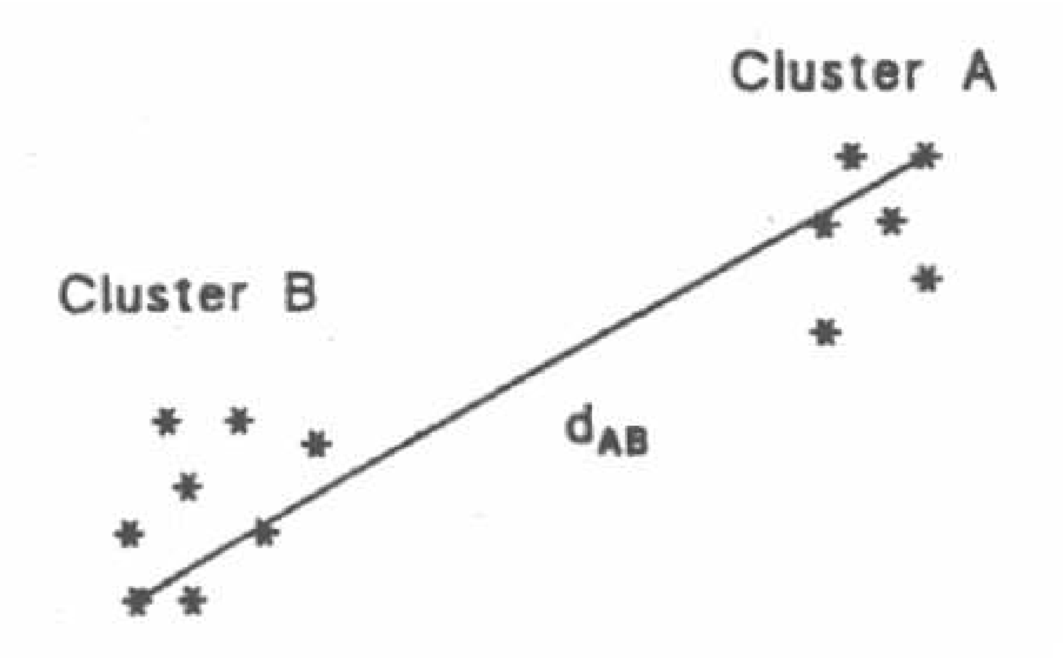
Single Linkage (SL) clustering

- We consider the distance between two clusters to be equal to the **shortest** distance from any member of one cluster to any member of the other one (**greatest** similarity).



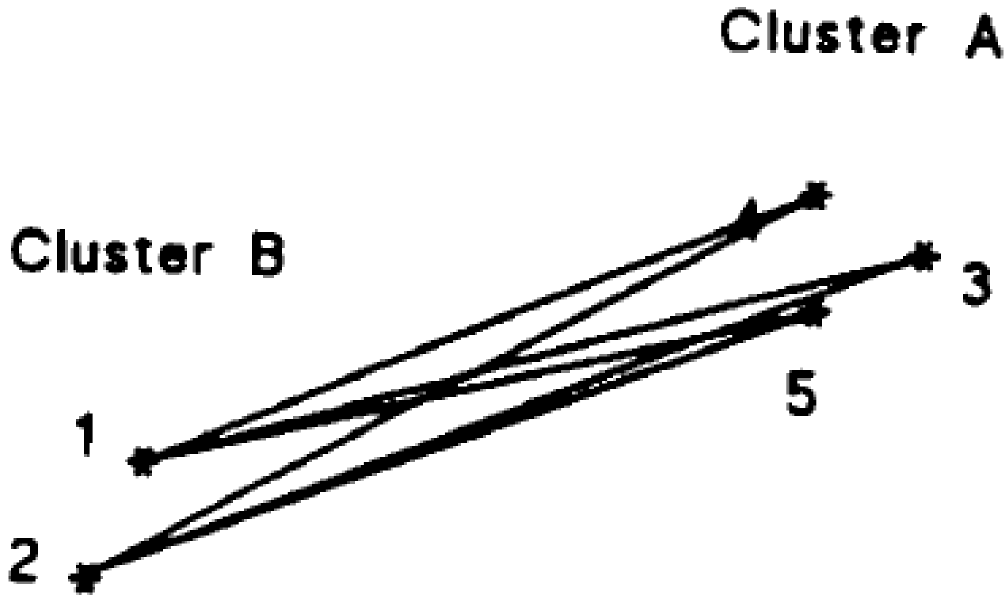
Complete Linkage (CL) clustering

- We consider the distance between two clusters to be equal to the **greatest** distance from any member of one cluster to any member of the other one (**smallest** similarity).



Group Average (GA) clustering

- We consider the distance between two clusters to be equal to the **average** distance from any member of one cluster to any member of the other one.



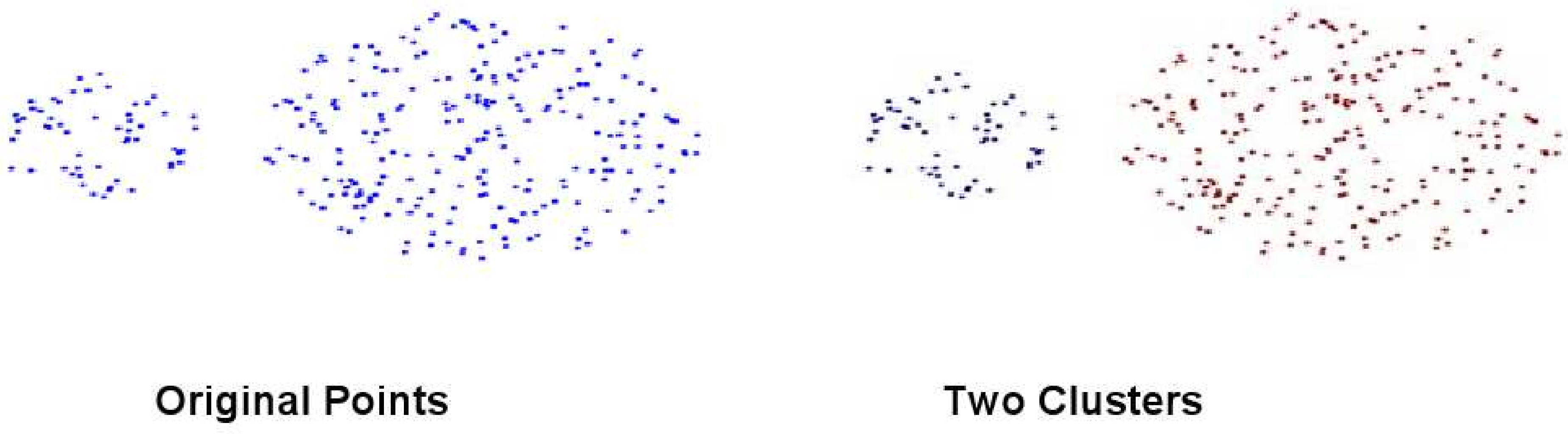
About distances

If the data exhibit strong clustering tendency, all 3 methods produce similar results.

- **SL**: requires only a single dissimilarity to be small. Drawback: produced clusters can violate the “compactness” property (cluster with large diameters)
- **CL**: opposite extreme (compact clusters with small diameters, but can violate the “closeness” property)
- **GA**: compromise, it attempts to produce relatively compact clusters and relatively far apart. BUT it depends on the dissimilarity scale.

Hierarchical algorithms limits

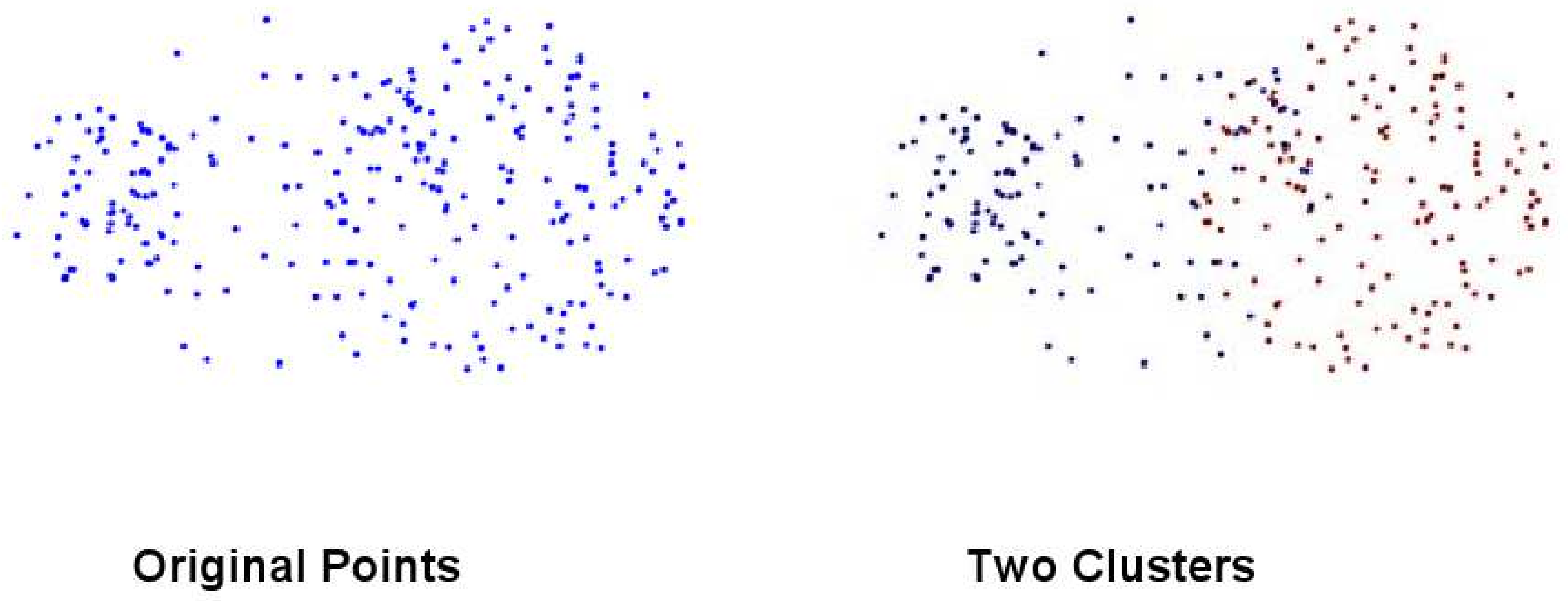
Strength of MIN



- Easily handles clusters of different sizes
- Can handle non elliptical shapes

Hierarchical algorithms limits

Limitations of MIN



- Sensitive to noise and outliers

Hierarchical algorithms limits

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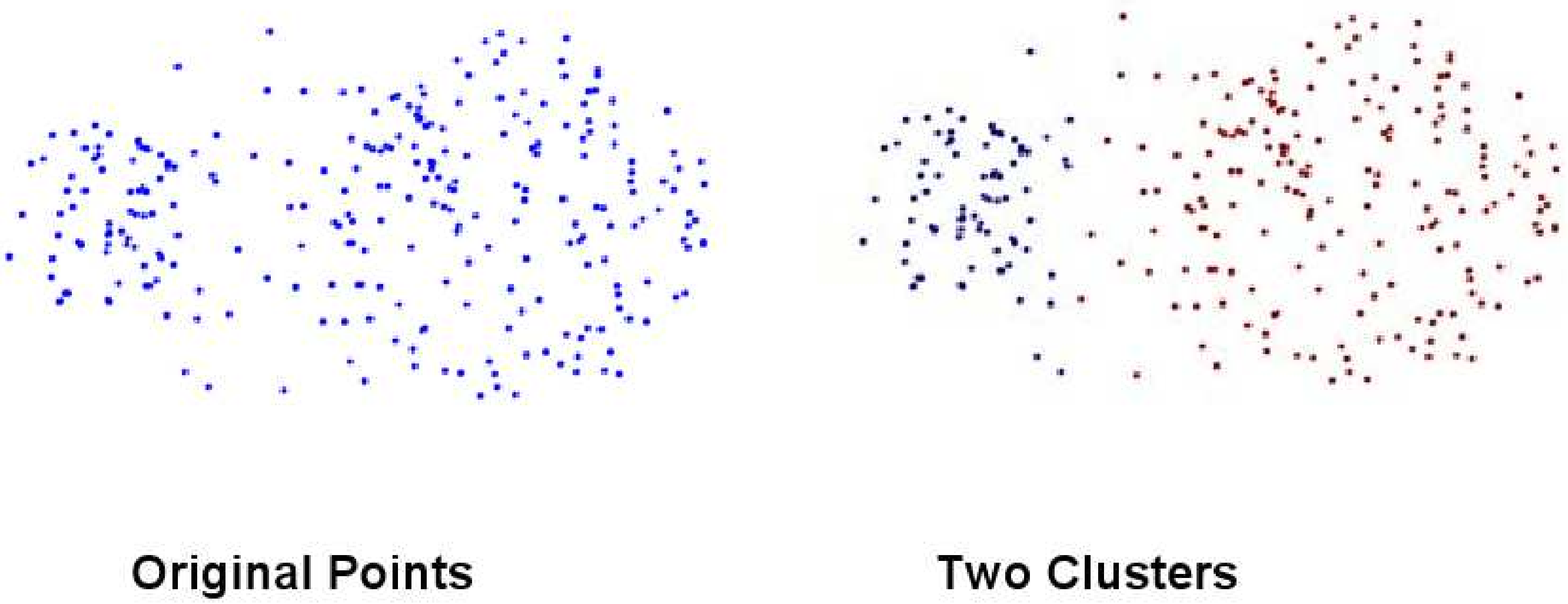
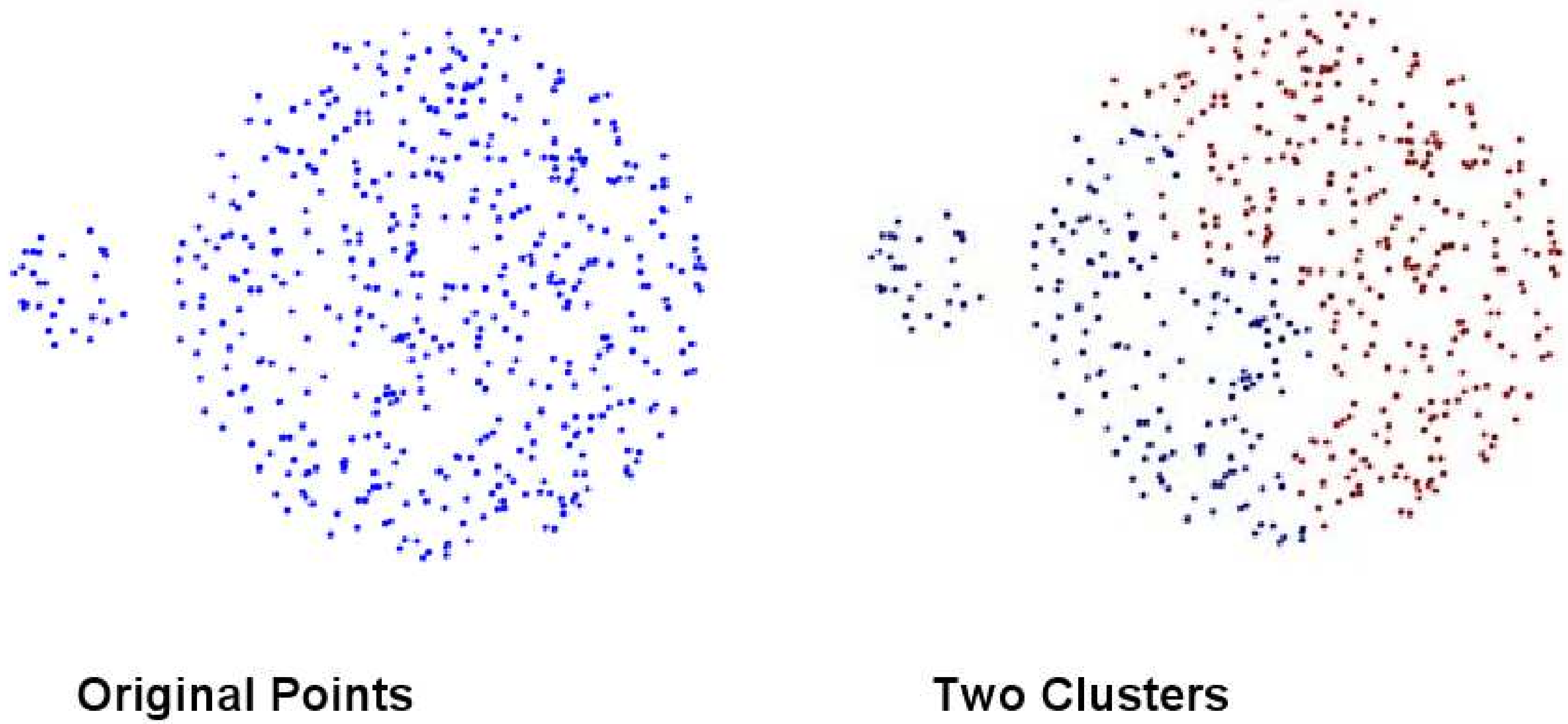


- Less sensible to noise and outliers

Hierarchical algorithms limits

Limitations of MAX



- Tends to break large clusters
- Biased toward globular clusters

Hierarchical clustering: Summary

- Advantages
  - It's nice that you get a hierarchy instead of an amorphous collection of groups
  - If you want k groups, just cut the $(k-1)$ longest links
- Disadvantages
  - It doesn't scale well: time complexity of at least $O(n^2)$, where n is the number of objects

Hierarchical Clustering Demo

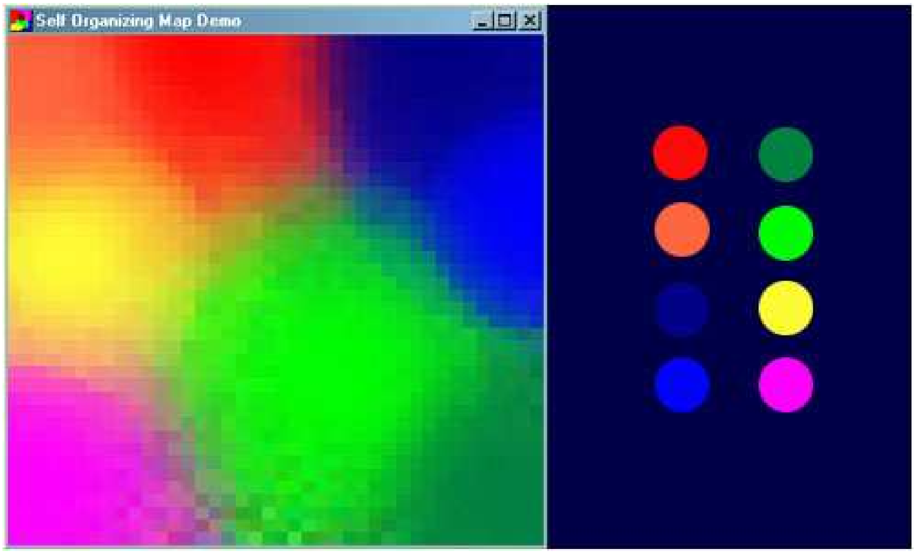
Time for another demo!

Self Organizing Features Maps

Kohonen Self Organizing Features Maps (a.k.a. SOM) provide a way to represent multidimensional data in much lower dimensional spaces.

- They implement a data compression technique similar to *vector quantization*
- They store information in such a way that any topological relationships within the training set are maintained

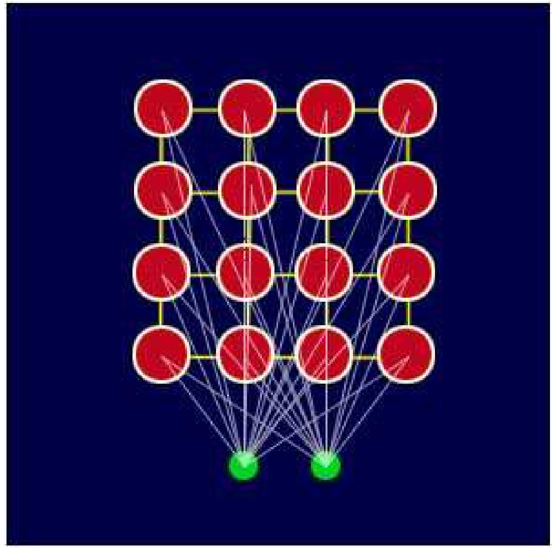
Example: Mapping of colors from their three dimensional components (i.e., red, green and blue) into two dimensions.



Self Organizing Feature Maps: The Topology

- The network is a lattice of "nodes", each of which is fully connected to the input layer
- Each node has a specific topological position and contains a vector of weights of the same dimension as the input vectors
- There are no lateral connections between nodes within the lattice

A SOM does not need a target output to be specified; instead, where the node weights match the input vector, that area of the lattice is selectively optimized to more closely resemble the data vector



Self Organizing Features Maps: The Algorithm

Training occurs in several steps over many iterations:

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6. Repeat step 2 for N iterations

Practical Learning of Self Organizing Features Maps

There are few things that have to be specified in the previous algorithm:

- Choosing the weights initialization

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$$||\mathbf{x} - \mathbf{w}_i|| = \sqrt{\sum_{k=1}^{p} (\mathbf{x}[k] - \mathbf{w}_i[k])^2}$$

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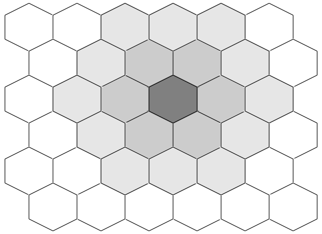

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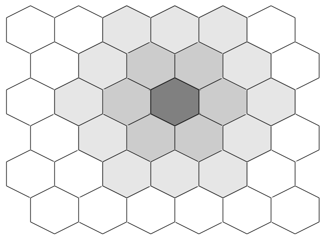

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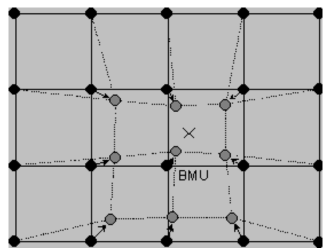
- Define the updating rule

$$\mathbf{w}_i(t+1) = \begin{cases} \mathbf{w}_i + \alpha(t)[\mathbf{x}(t) - \mathbf{w}_i(t)], & i \in N_i(t) \\ \mathbf{w}_i, & i \notin N_i(t) \end{cases}$$



Self Organizing Feature Maps Demo

Stolen from:
http://www.ai-junkie.com

Bibliography

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- K-means and Hierarchical Clustering
  Tutorial Slides by A. Moore
- "Metodologie per Sistemi Intelligenti" course - Clustering
  Tutorial Slides by P.L. Lanzi
- K-Means Clustering Tutorials
  Online tutorials by K. Teknomo
- As usual, more info on del.icio.us

- The end