ICSI431/ICSI531 Data Mining
Lecture 5
Clustering

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Slides adapted from David Sontag, Luke Zettlemoyer, Vibhav Gogate, Carlos Guestrin, Andrew Moore, Dan Klein, Pang-Ning Tan, Michael Seinbach, Vipin Kumar

Outline

- Introduction
- Cluster Methods
  - K-Means
  - Agglomerative (Hierarchical) Clustering
- Cluster Validation

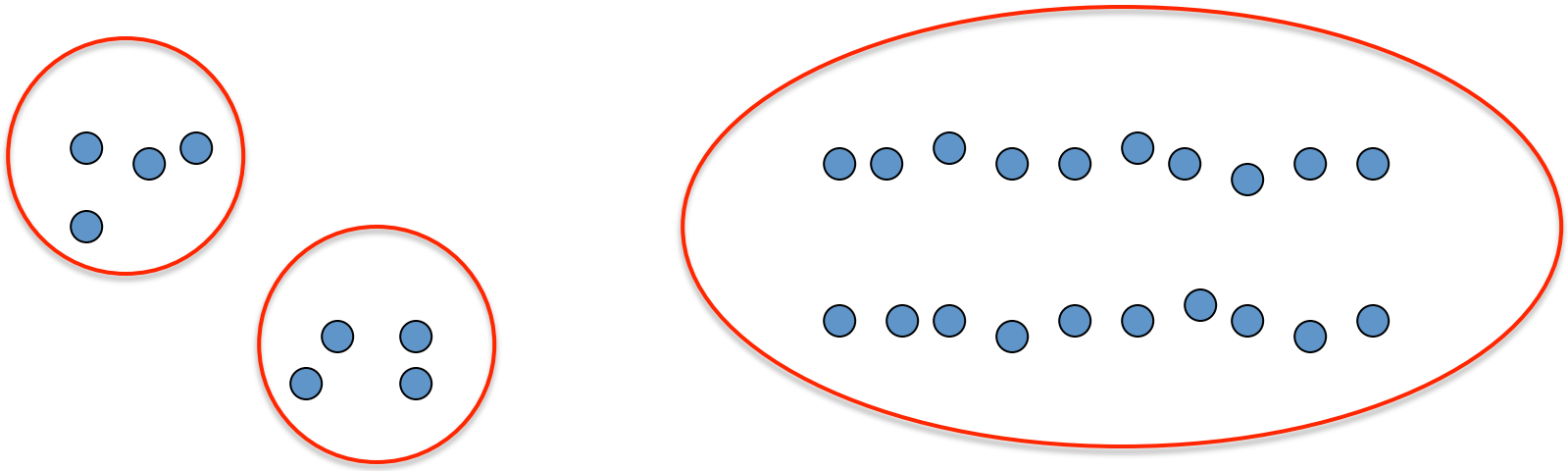
Clustering

Clustering:

- Unsupervised learning
- Requires data, but no labels
- Detect patterns e.g. in
  - Group emails or search results
  - Customer shopping patterns
  - Regions of images
- Useful when don't know what you're looking for
- But: can get gibberish

Clustering

- Basic idea: group together similar instances
- Example: 2D point patterns



Clustering

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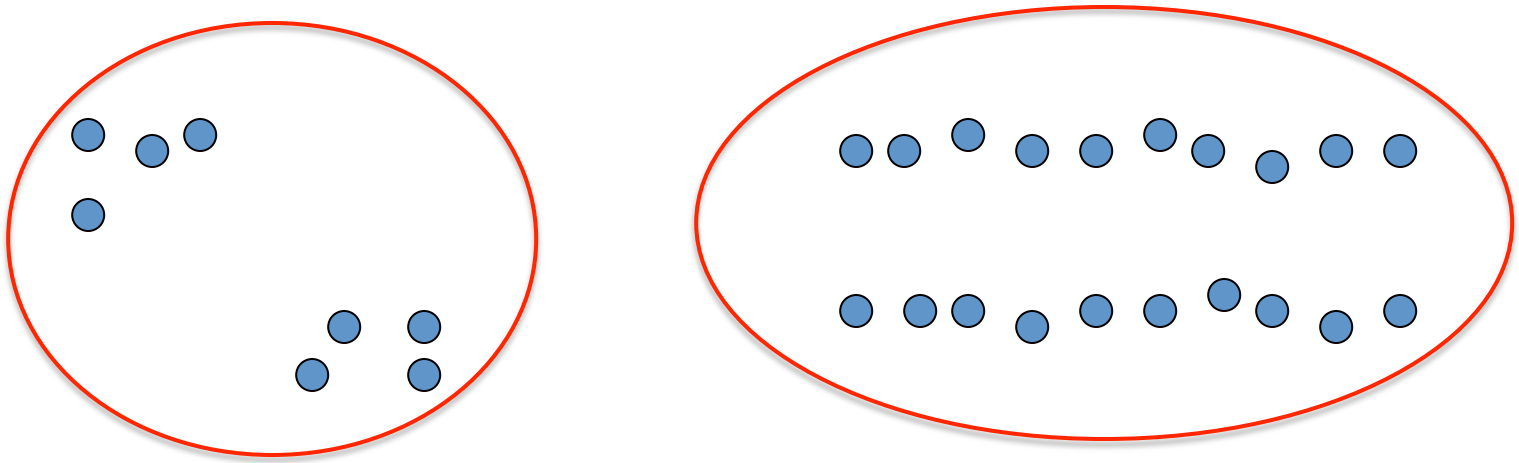

Clustering

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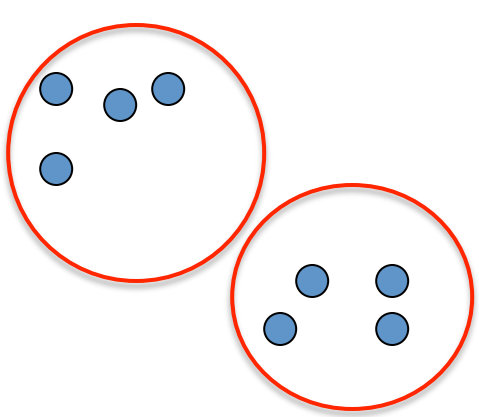
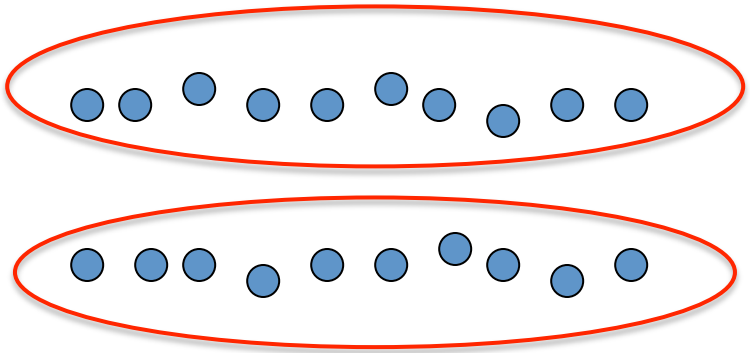
- Example: 2D point patterns





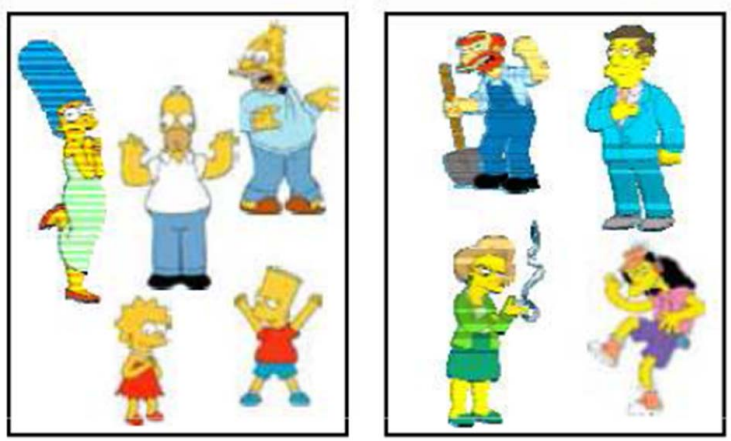
- What could "similar" mean?
  - One option: small Euclidean distance (squared)

$$\mathrm{dist}(\vec{x}, \vec{y}) = ||\vec{x} - \vec{y}||_2^2$$

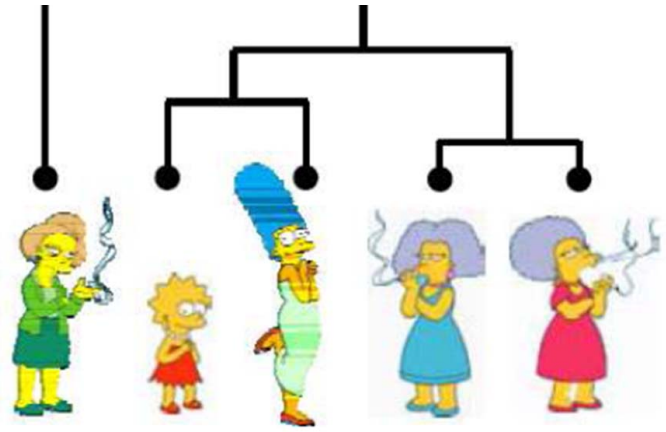
  - Clustering results are crucially dependent on the measure of similarity (or distance) between "points" to be clustered

Clustering algorithms

- Partition algorithms (Flat)
  - K-means
  - Mixture of Gaussian
  - Spectral Clustering



- Hierarchical algorithms
  - Bottom up – agglomerative
  - Top down – divisive



Clustering examples

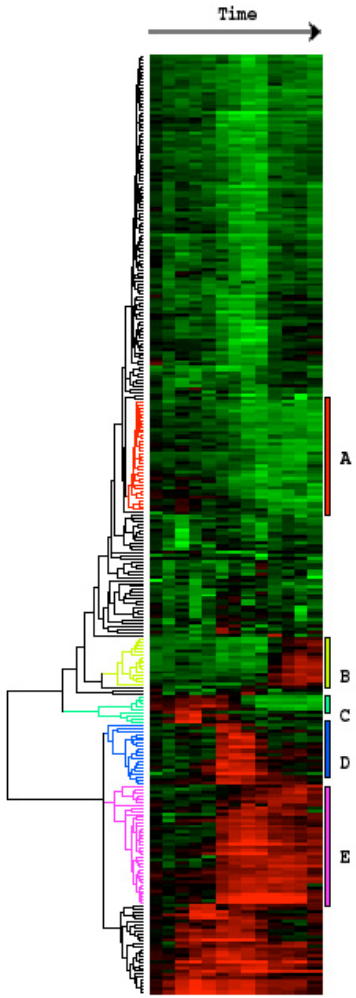
Image segmentation

Goal: Break up the image into meaningful or perceptually similar regions

[Slide from James Hayes]

Clustering examples

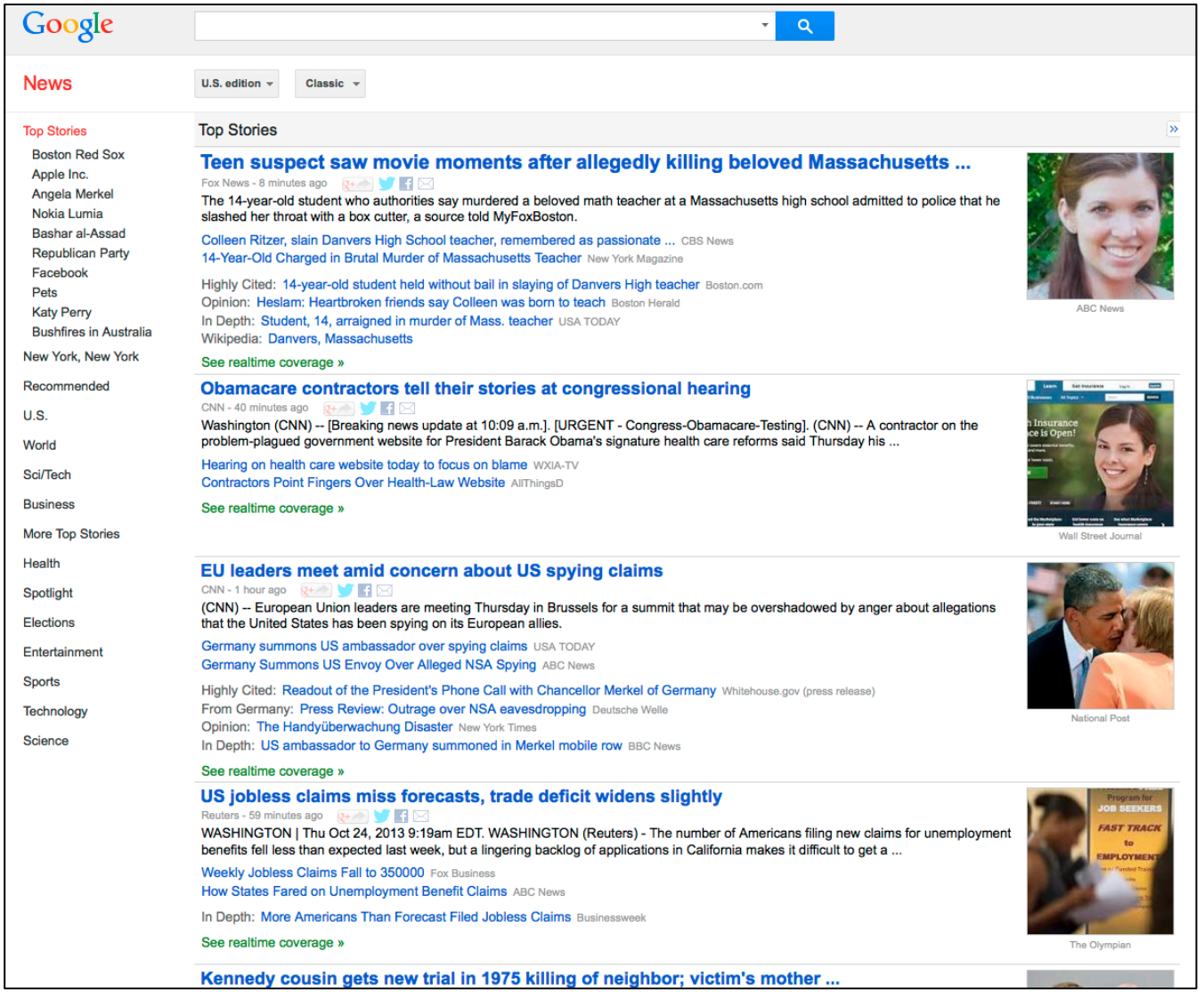
Clustering gene expression data



Eisen et al, PNAS 1998

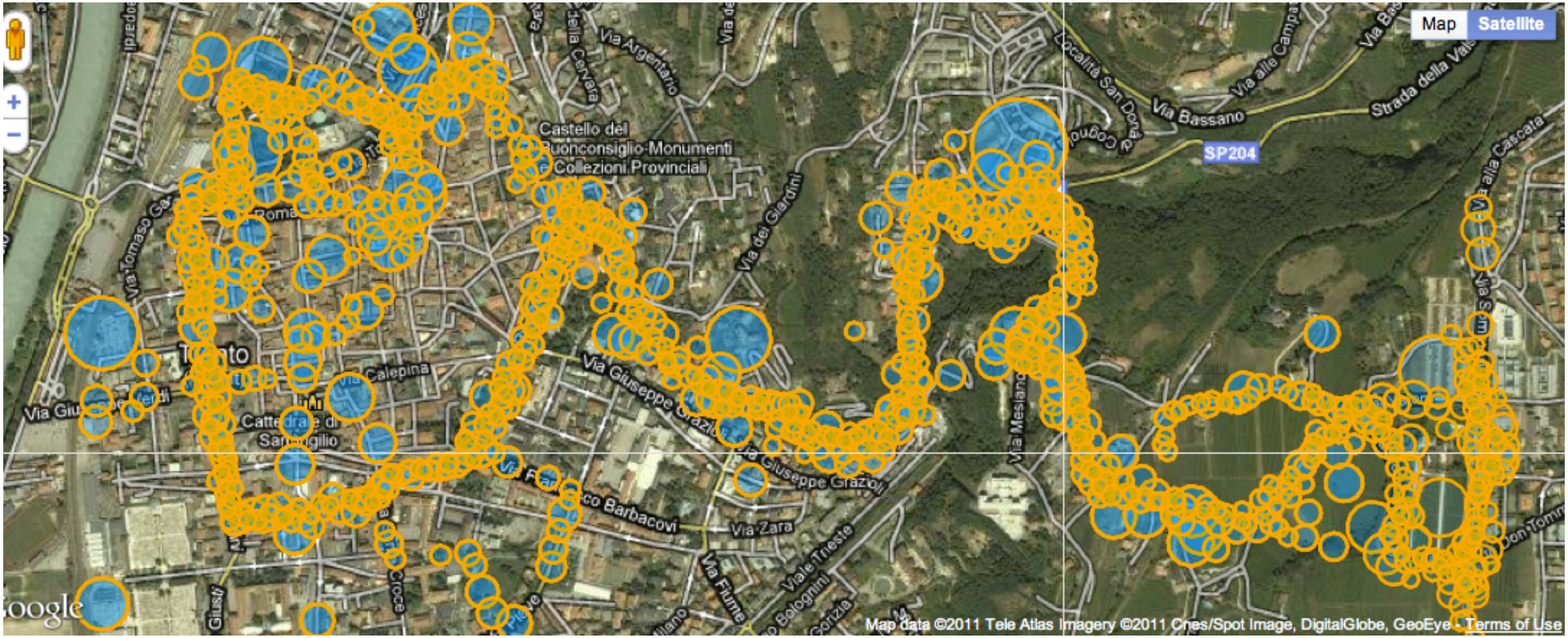
Clustering examples

Cluster news articles



Clustering examples

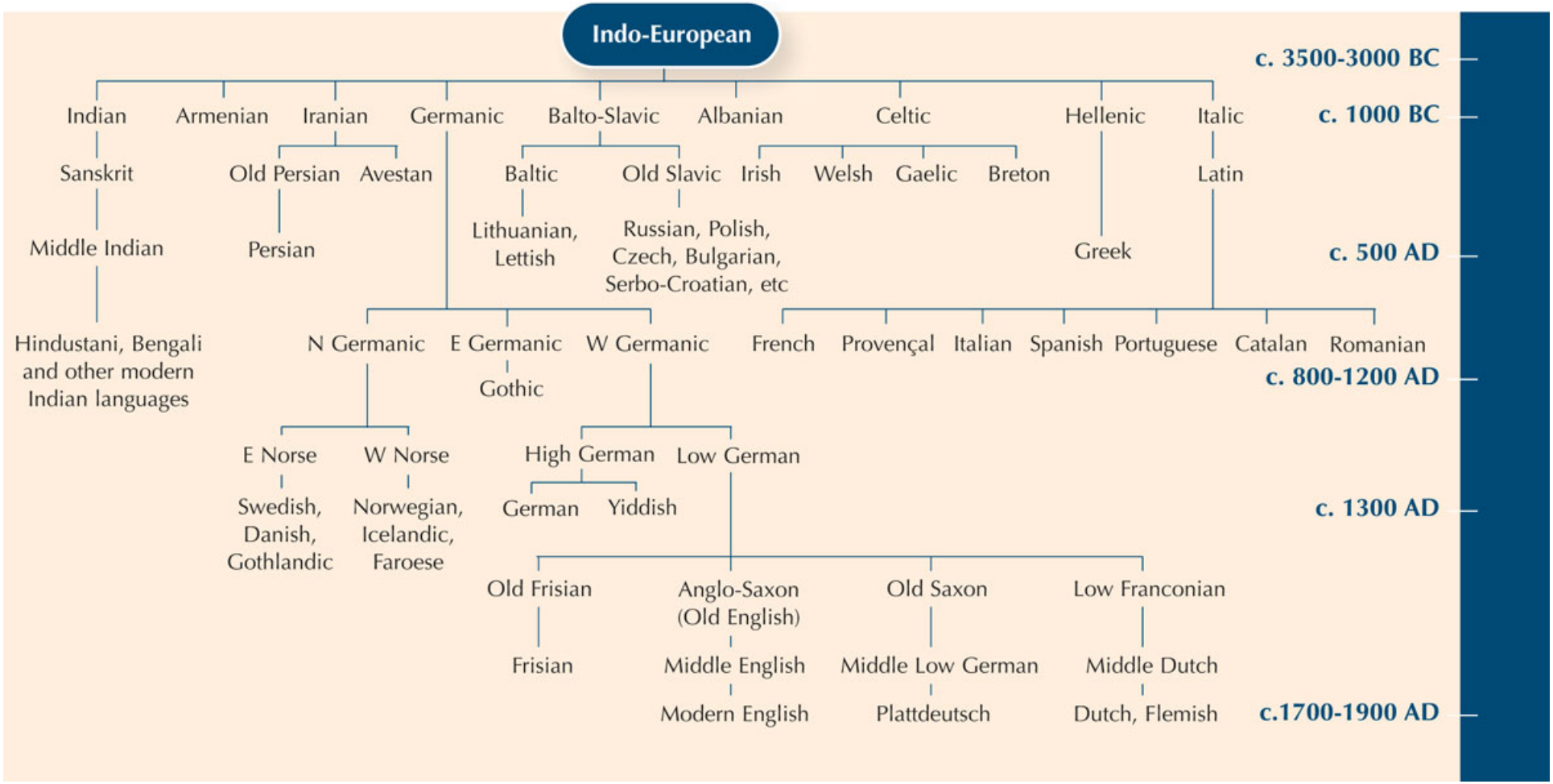
Cluster people by space and time



[Image from Pilho Kim]

Clustering examples

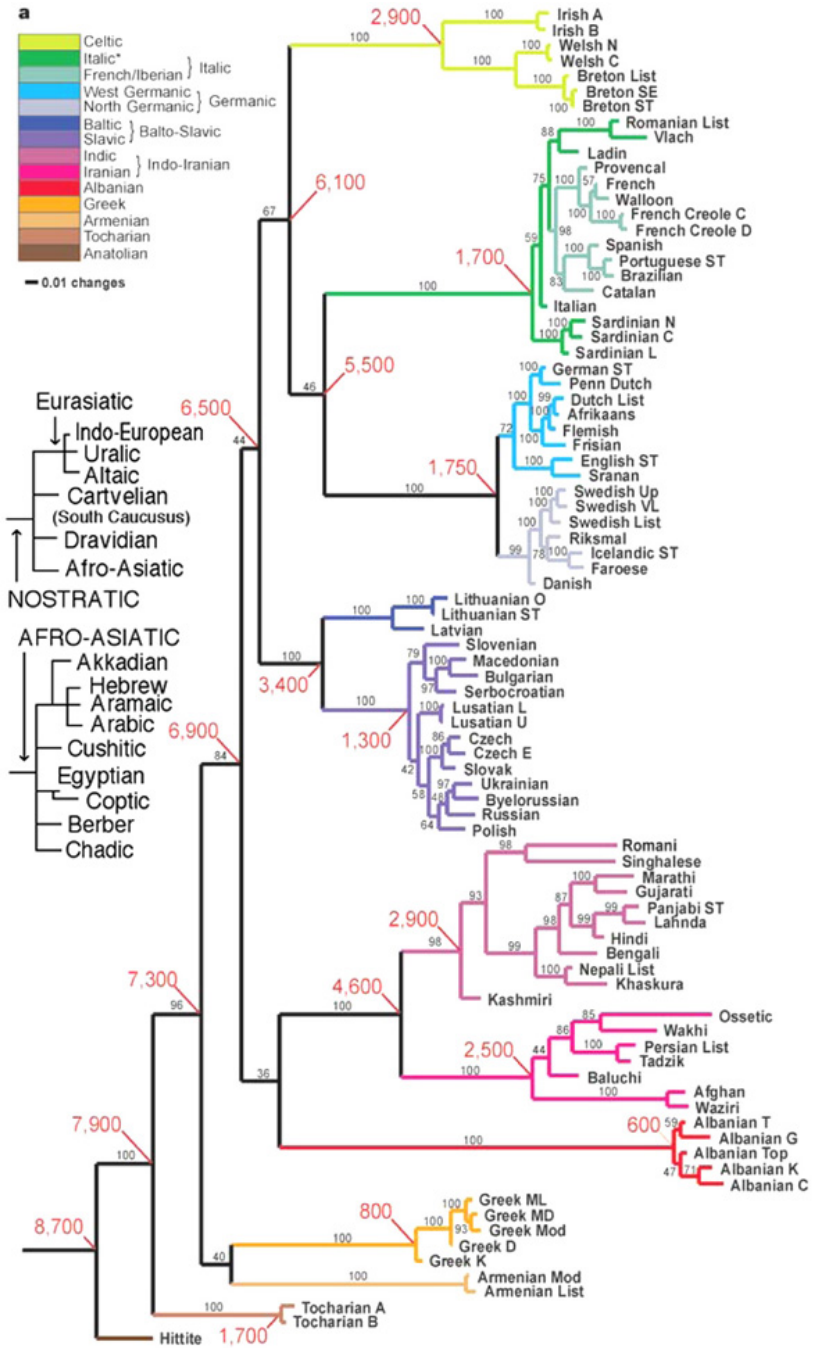
Clustering languages



[Image from scienceinschool.org]

Clustering examples

Clustering languages

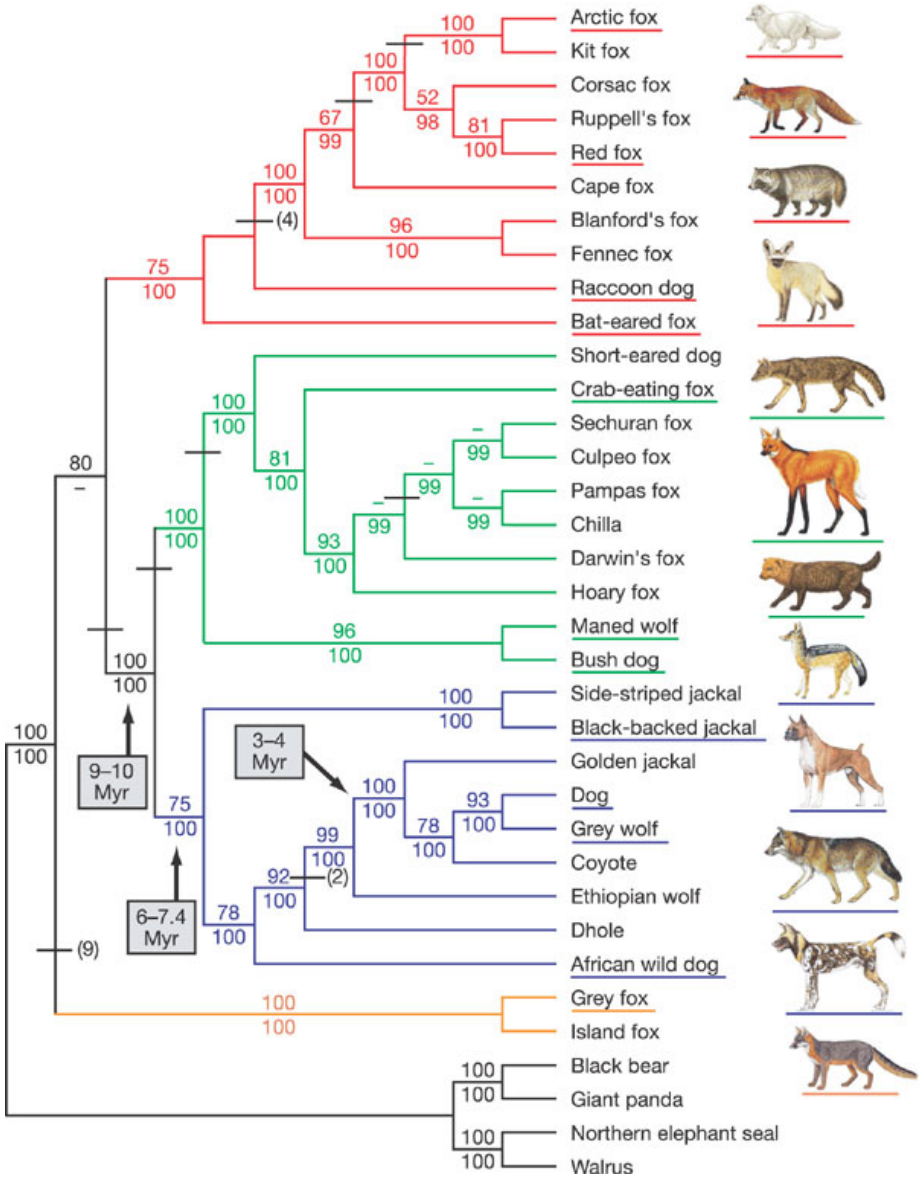


[Image from dhushara.com]

Clustering examples

Clustering species

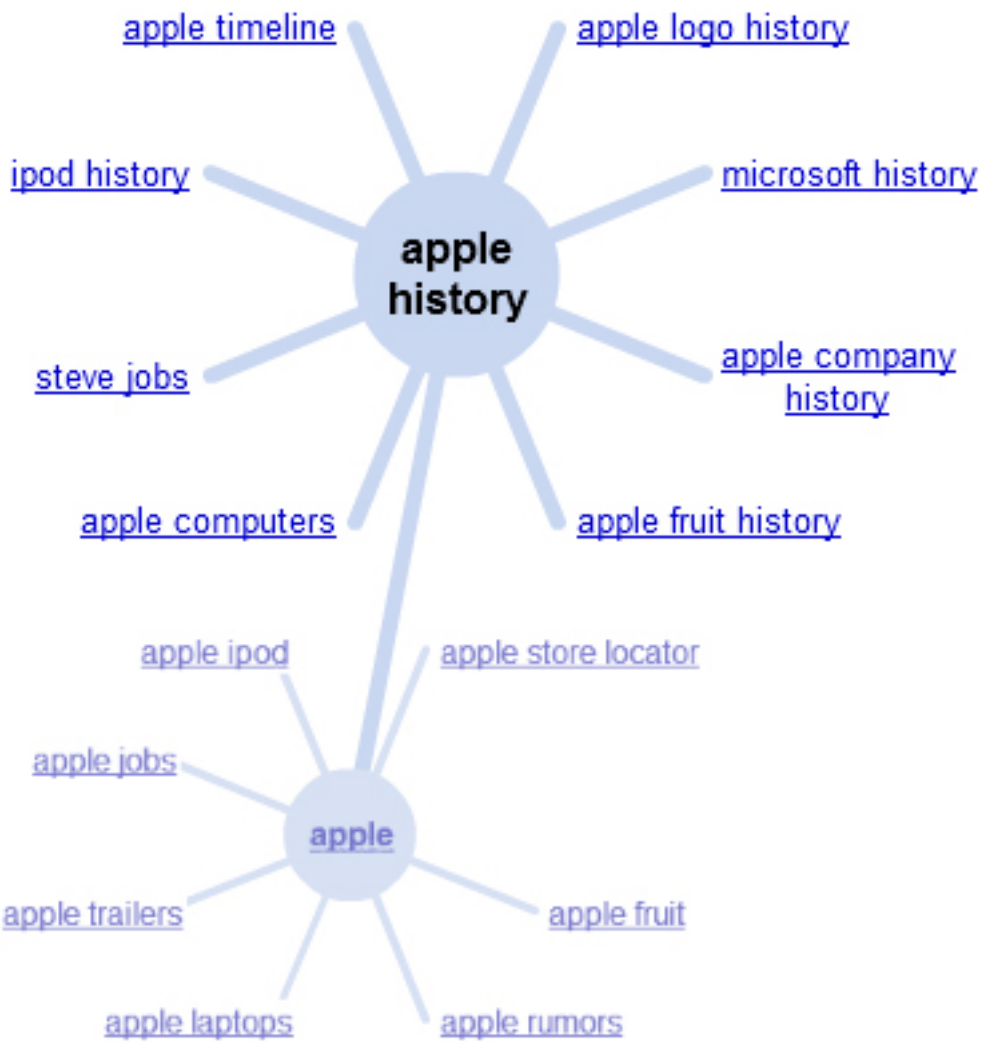
(“phylogeny”)



[Lindblad-Toh et al., Nature 2005]

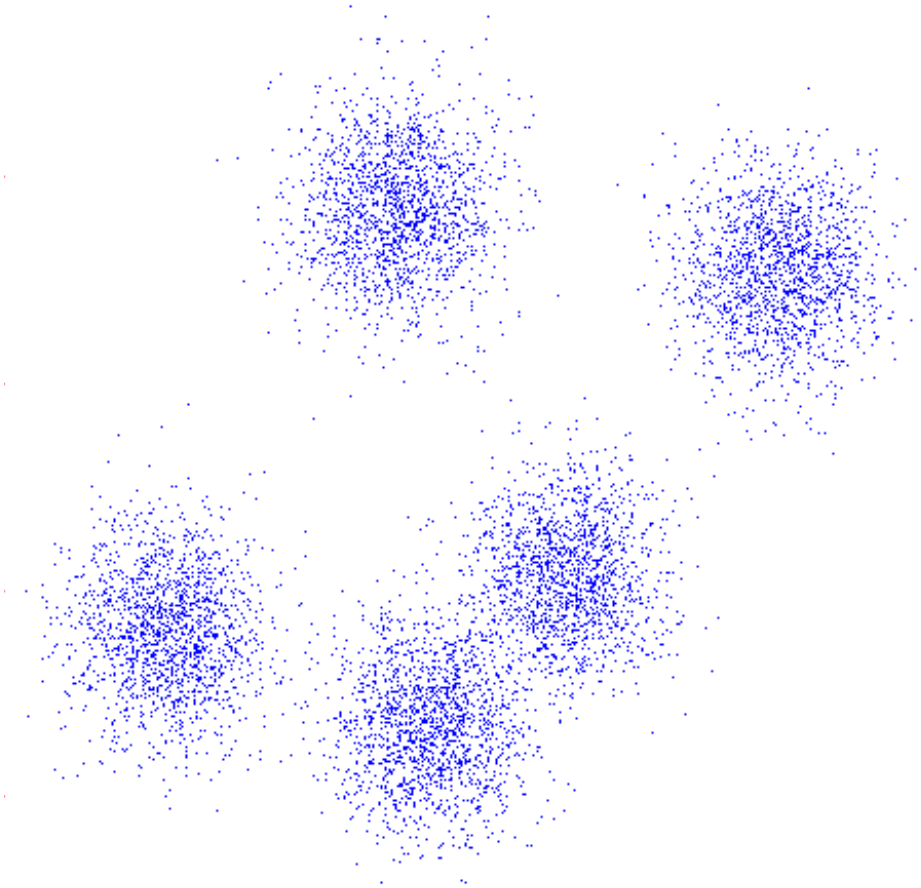
Clustering examples

Clustering search queries



K-Means

- An iterative clustering algorithm
  - Initialize: Pick *K* random points as cluster centers
  - Alternate:
    1. Assign data points to closest cluster center
    2. Change the cluster center to the average of its assigned points
  - Stop when no points' assignments change



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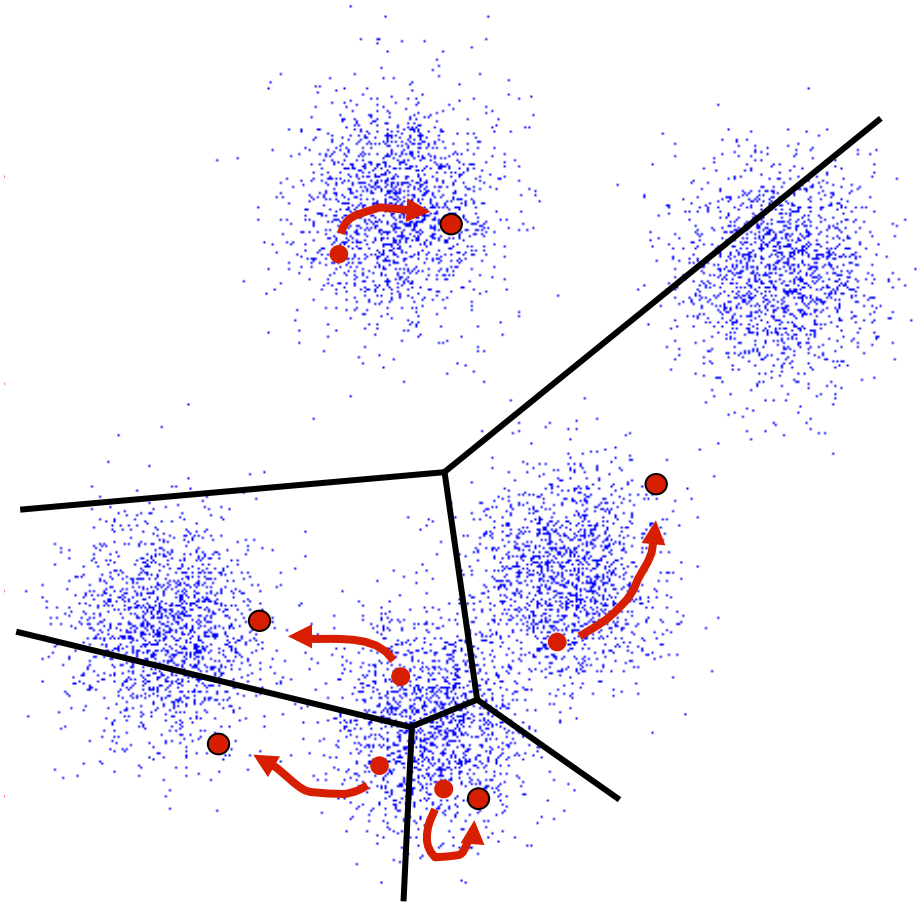
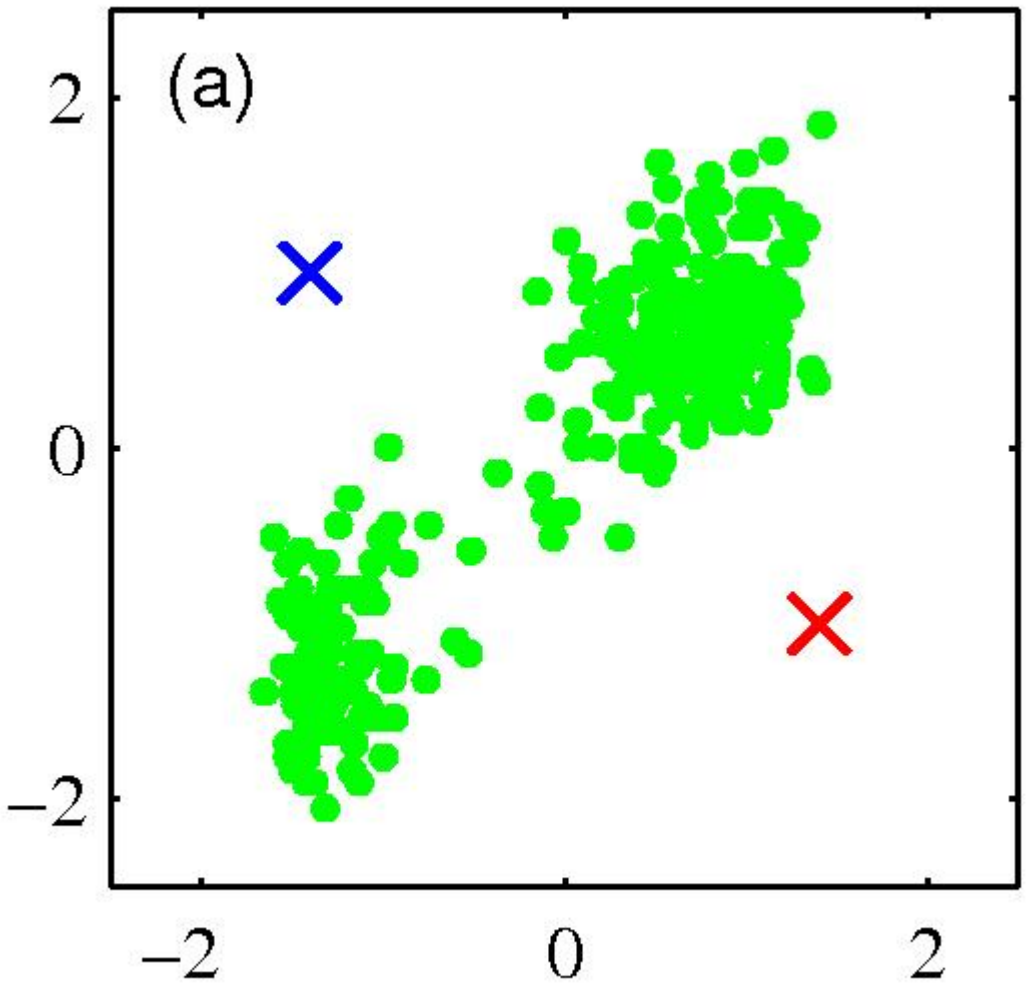


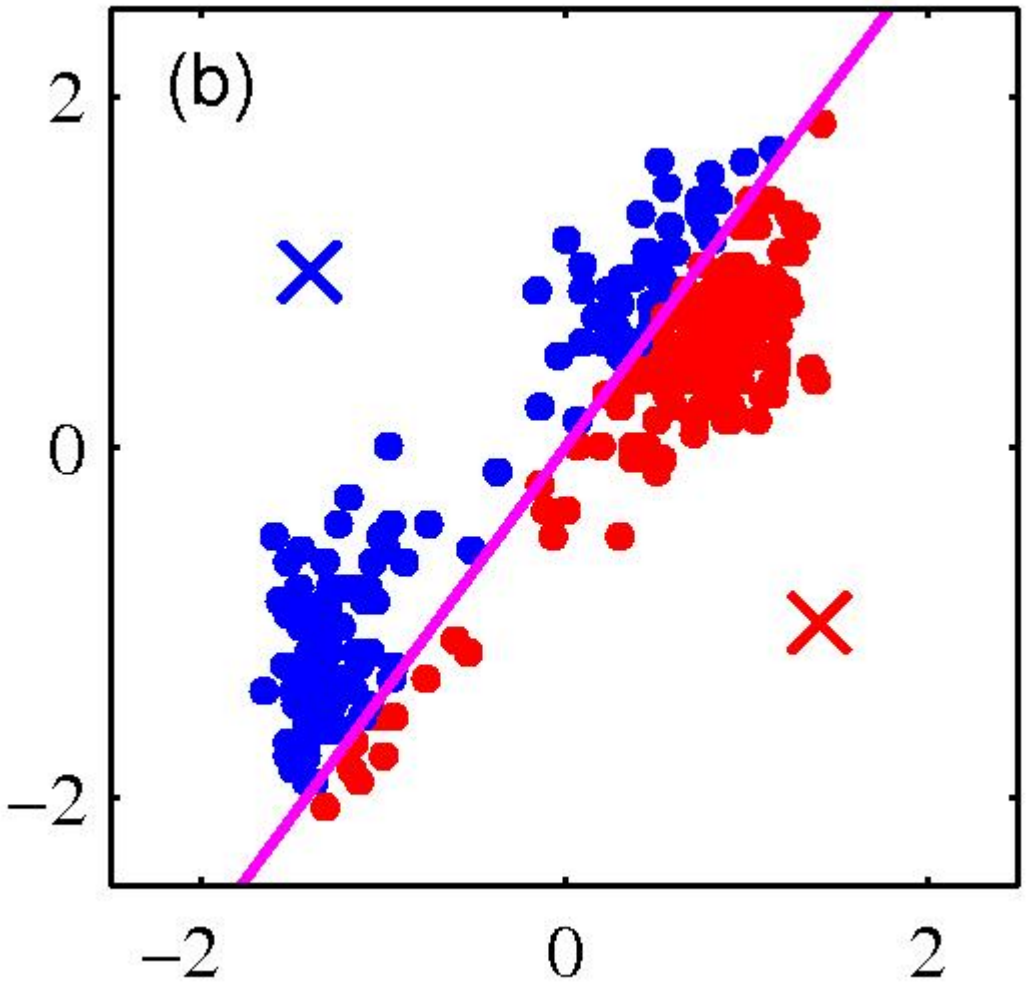
K-means clustering: Example



- Pick *K* random points as cluster centers (means)

Shown here for *K*=2

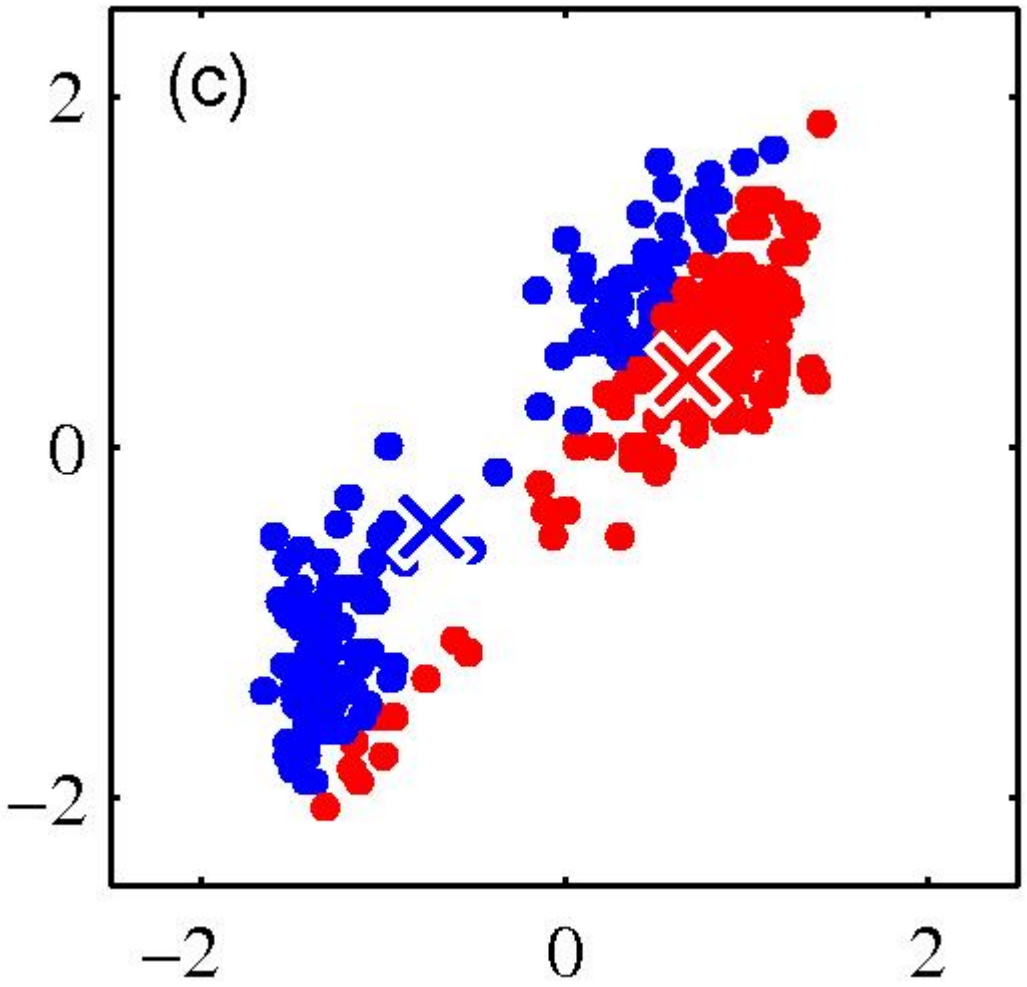
K-means clustering: Example



Iterative Step 1

- Assign data points to closest cluster center

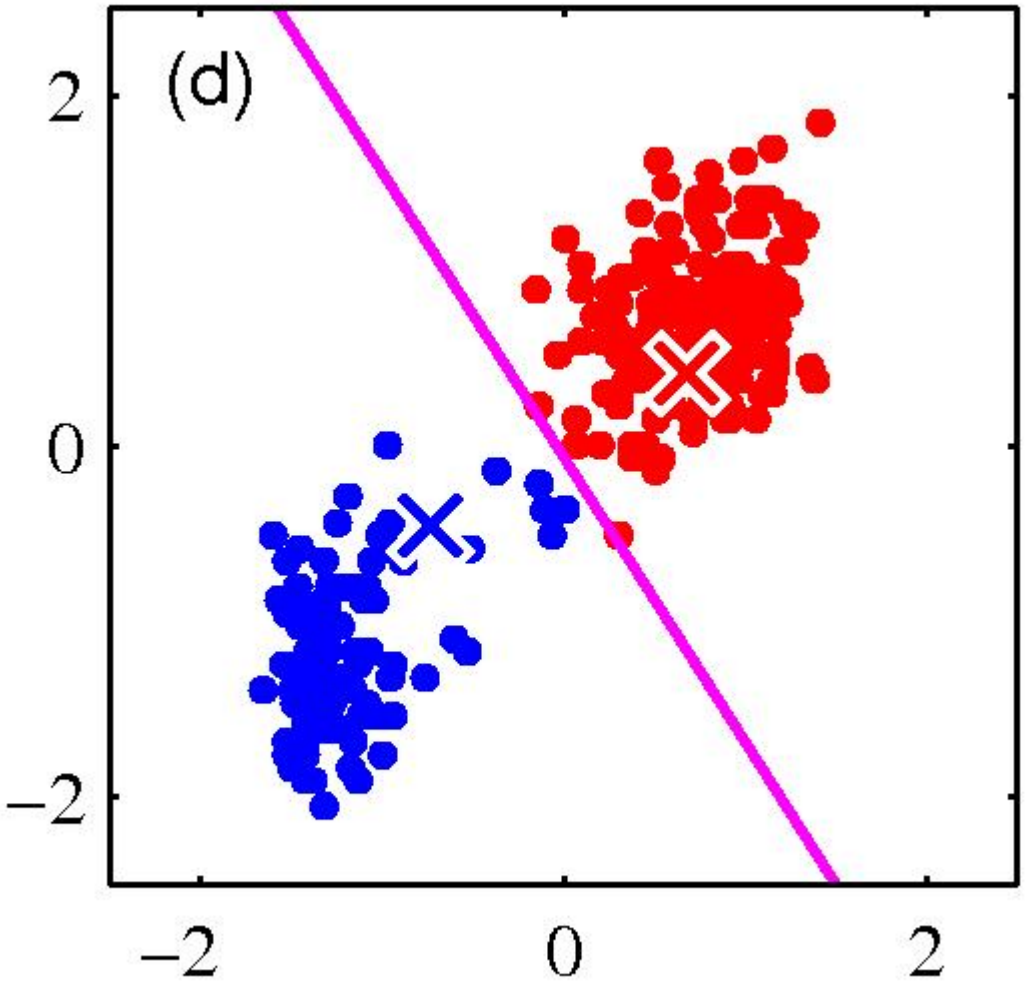
K-means clustering: Example



Iterative Step 2

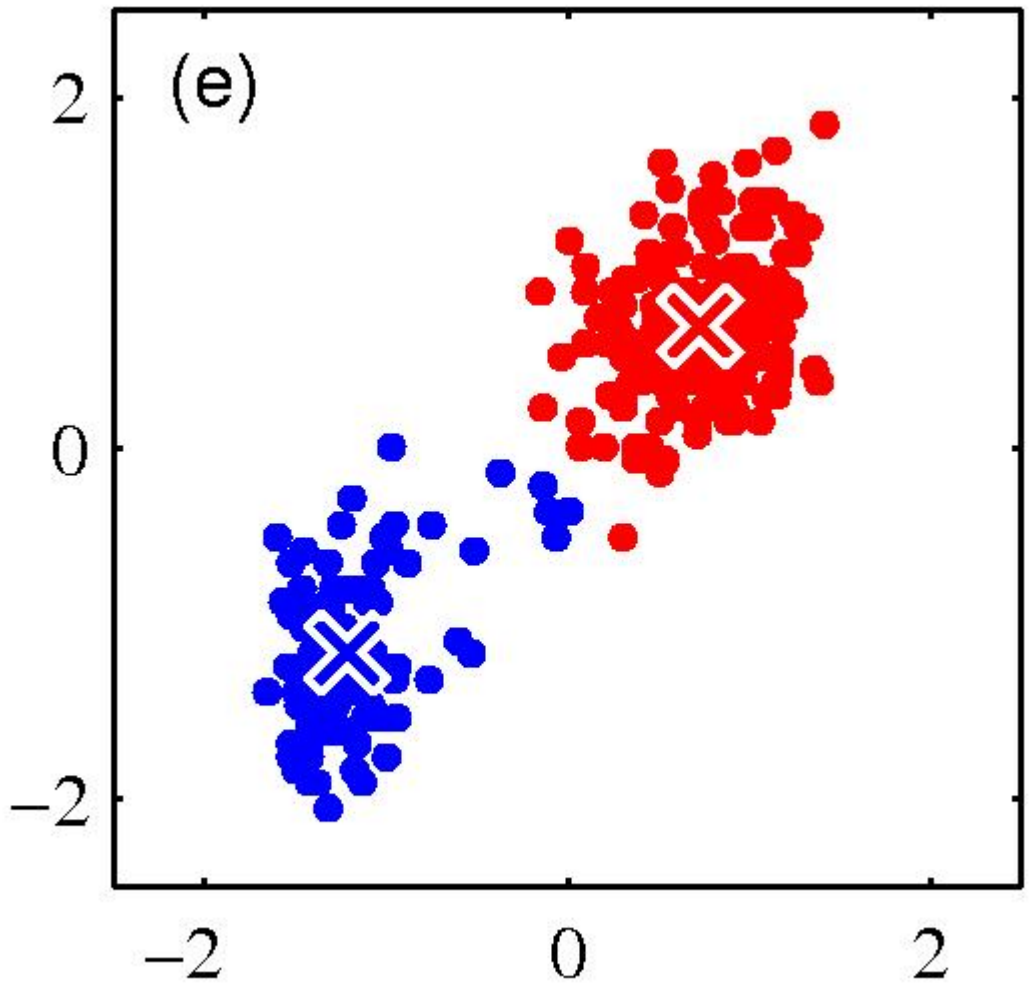
- Change the cluster center to the average of the assigned points

K-means clustering: Example

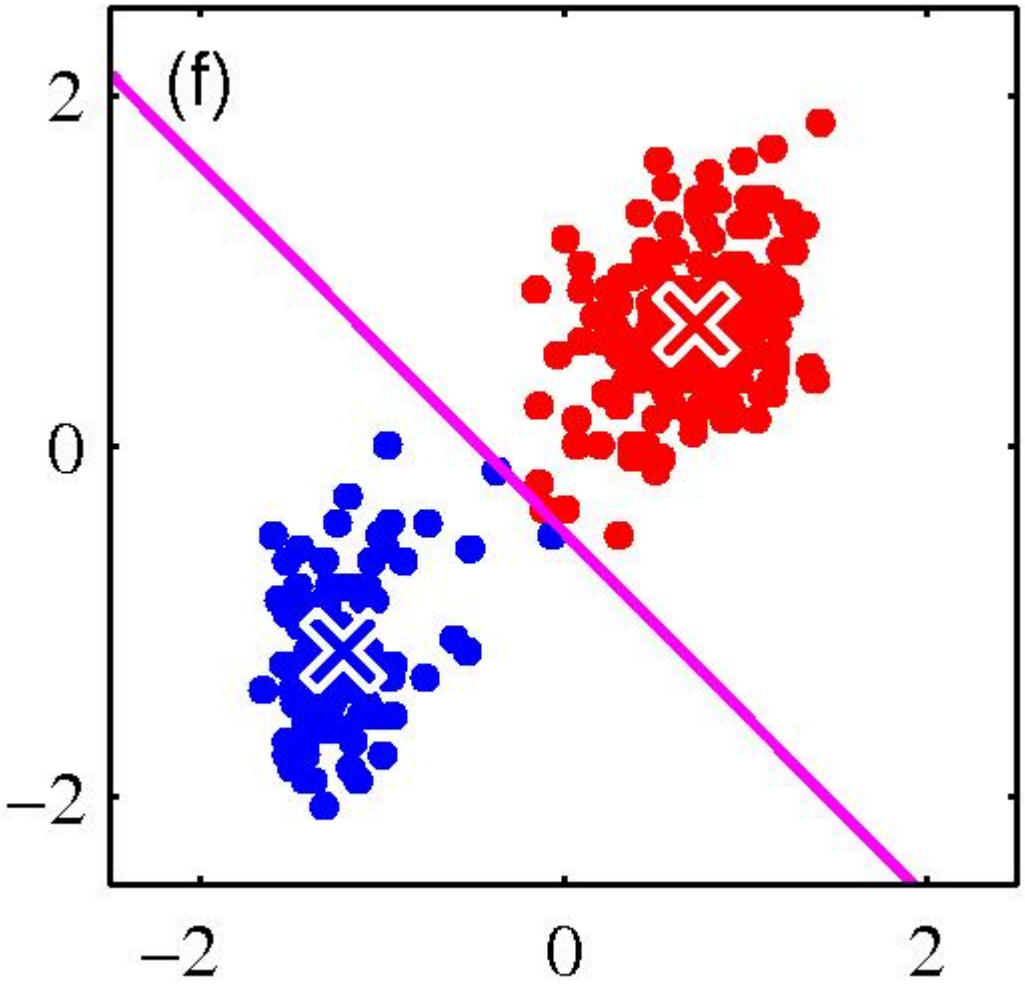


- Repeat until convergence

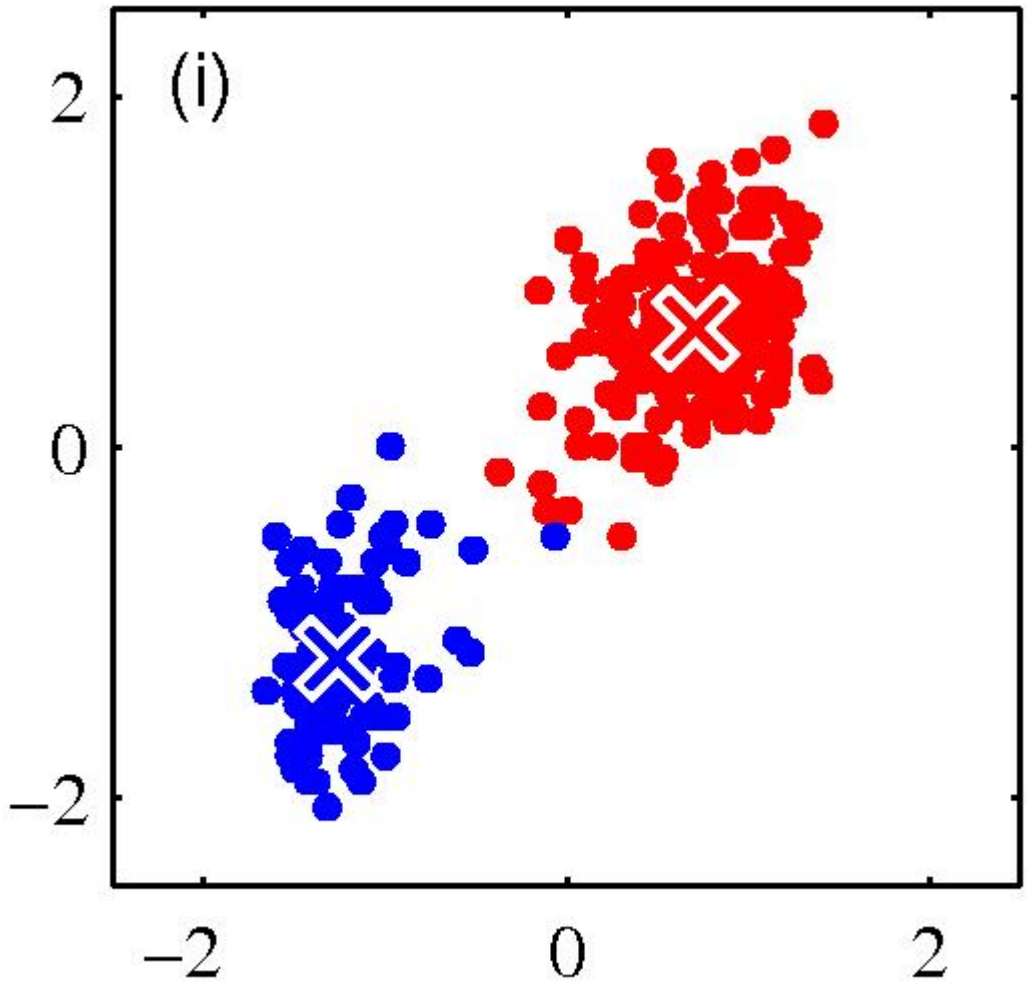
K-means clustering: Example



K-means clustering: Example



K-means clustering: Example



Properties of K-means **algorithm**

- Guaranteed to converge in a finite number of iterations

- Running time per iteration:
    1. Assign data points to closest cluster center

       O(KN) time

    2. Change the cluster center to the average of its assigned points

       O(N)

Example: K-Means for Segmentation

K=2

Goal of Segmentation is to partition an image into regions each of which has reasonably homogenous visual appearance.

Original

Example: K-Means for Segmentation

K=2

K=3

Original

Example: K-Means for Segmentation

K=2

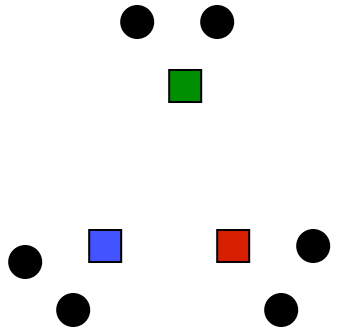
K=3

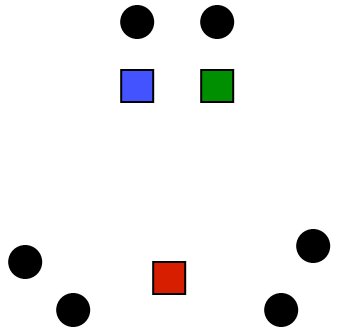
K=10

Original

Initialization

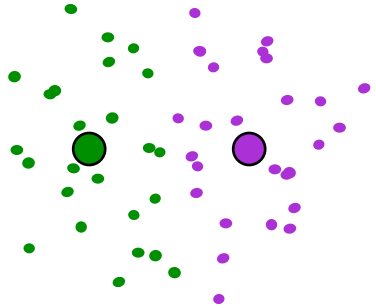
- K-means **algorithm** is a heuristic
  - Requires initial means
  - It does matter what you pick!
  - What can go wrong?
  - Various schemes for preventing this kind of thing: variance-based split / merge, initialization heuristics



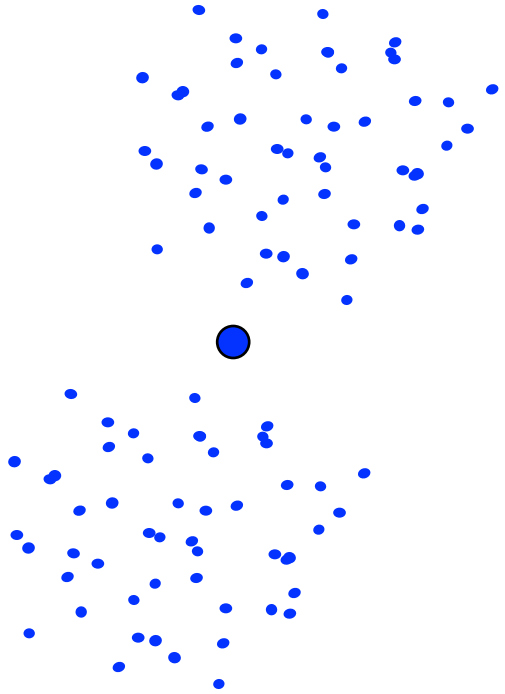


K-Means Getting Stuck

A local optimum:

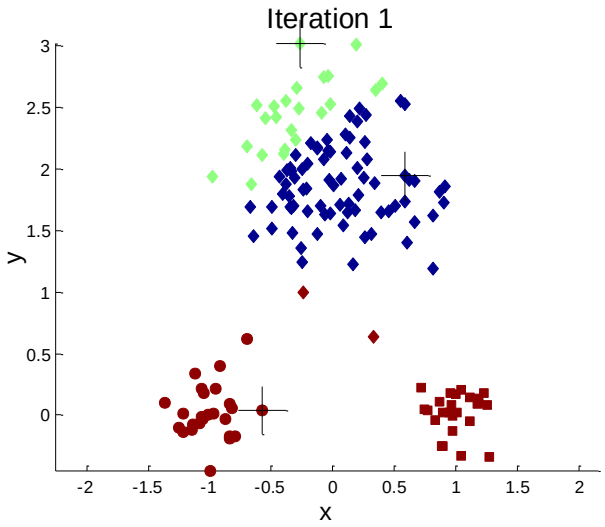


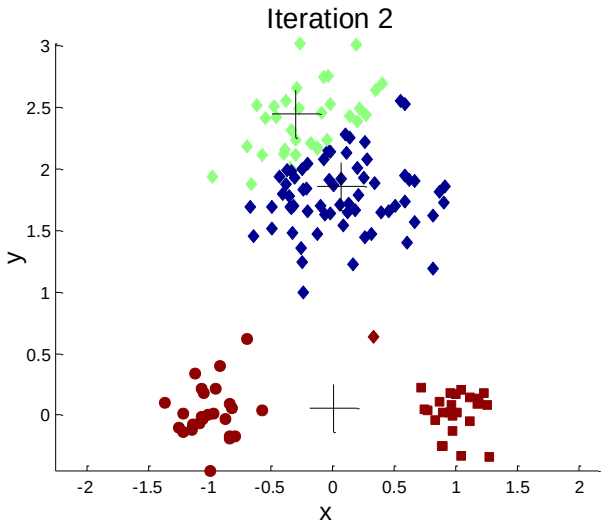
Would be better to have
one cluster here

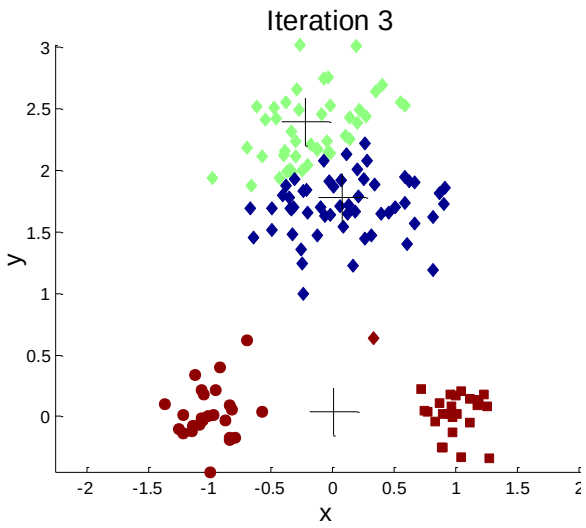


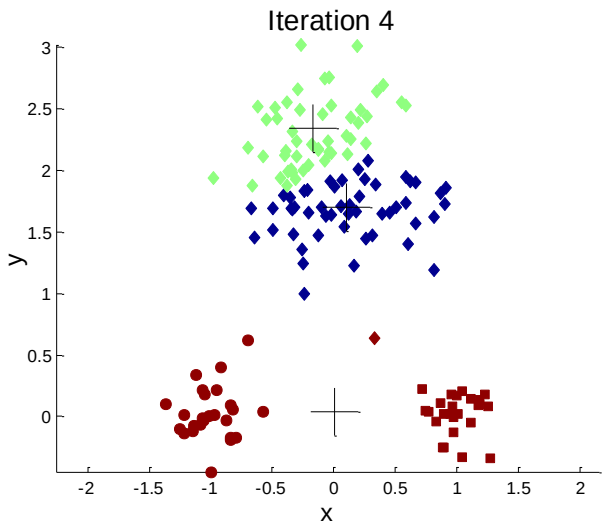
… and two clusters here

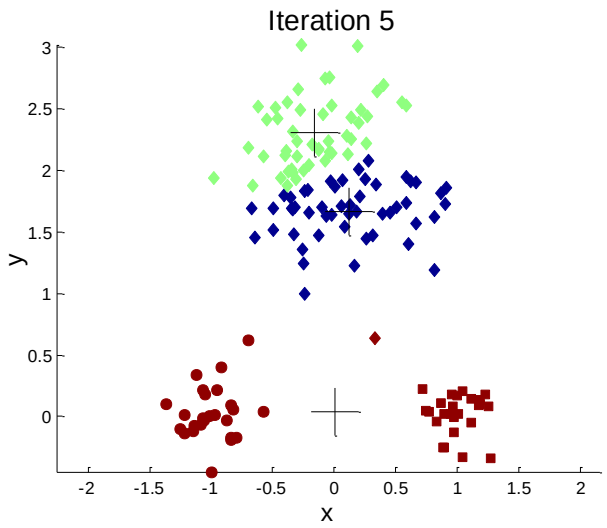
Example: bad initial centroids



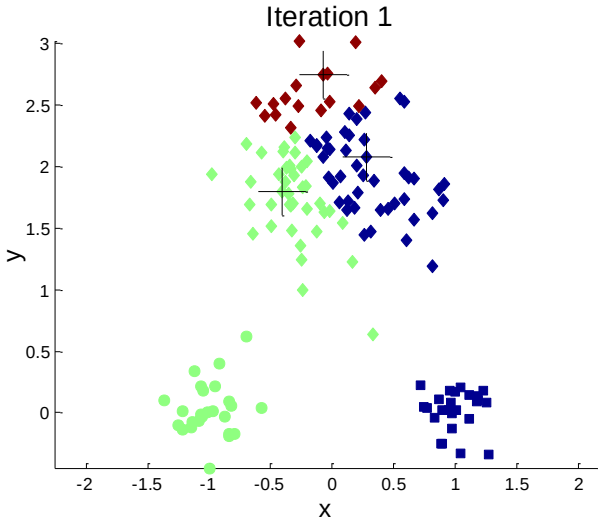


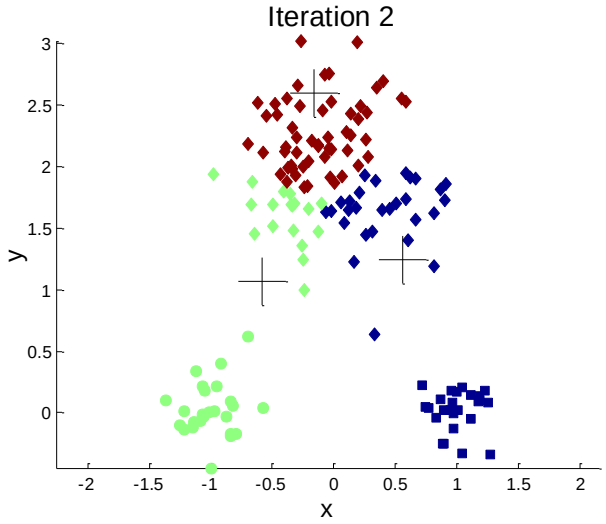


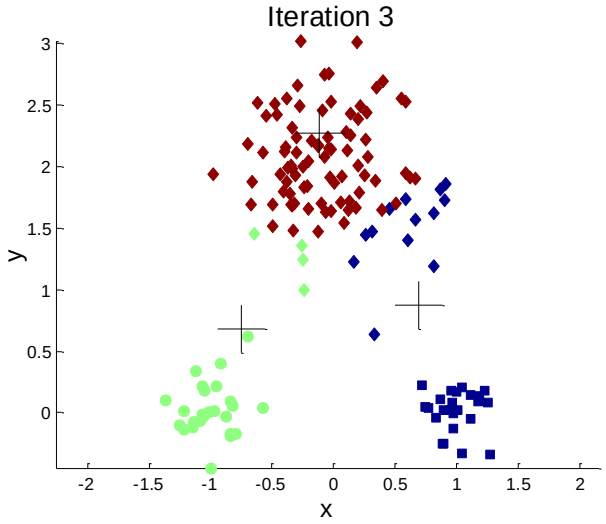


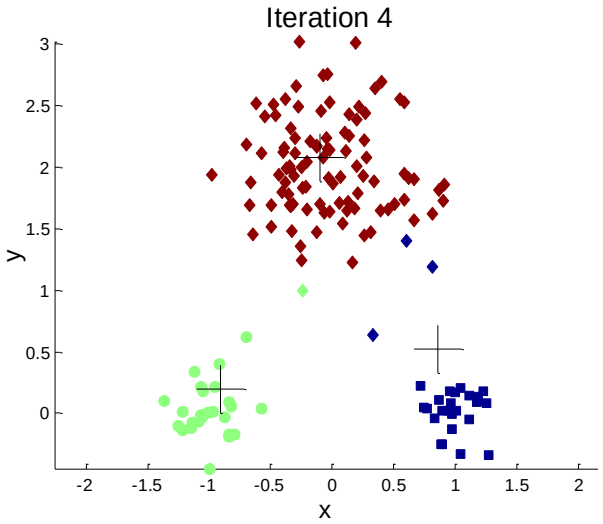


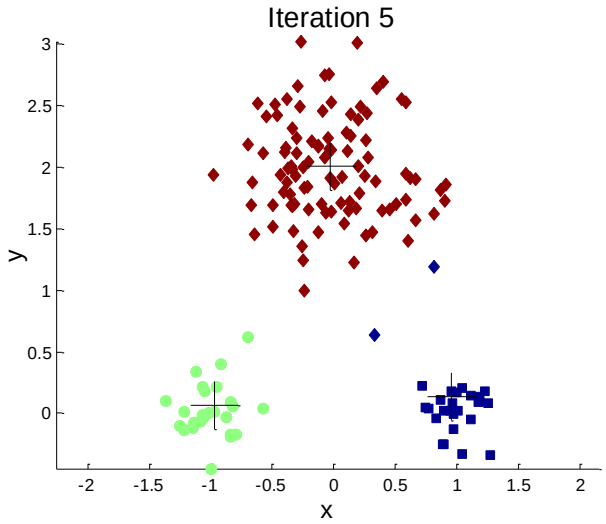
Example: good initial centroids

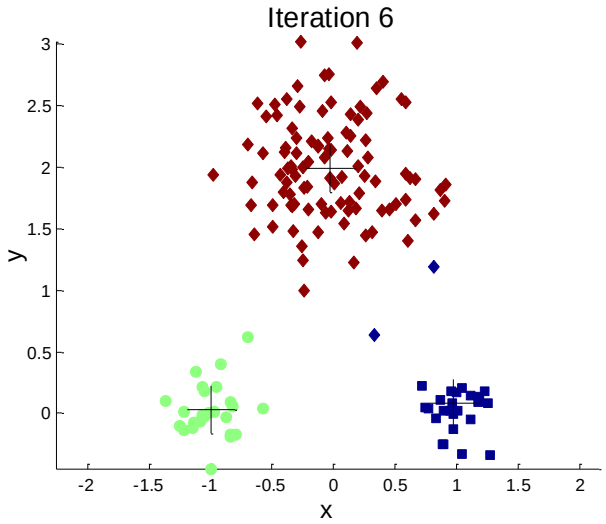




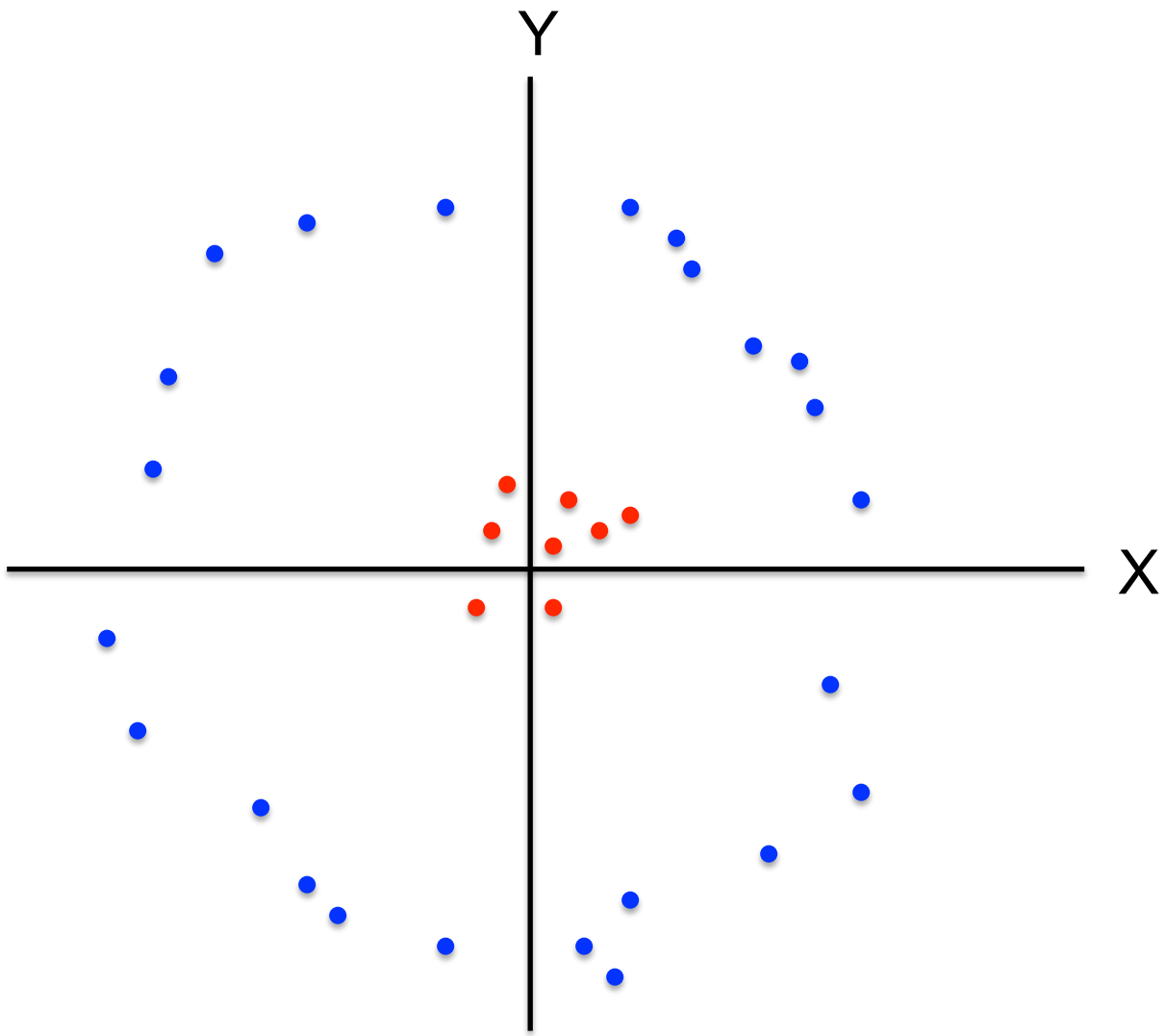




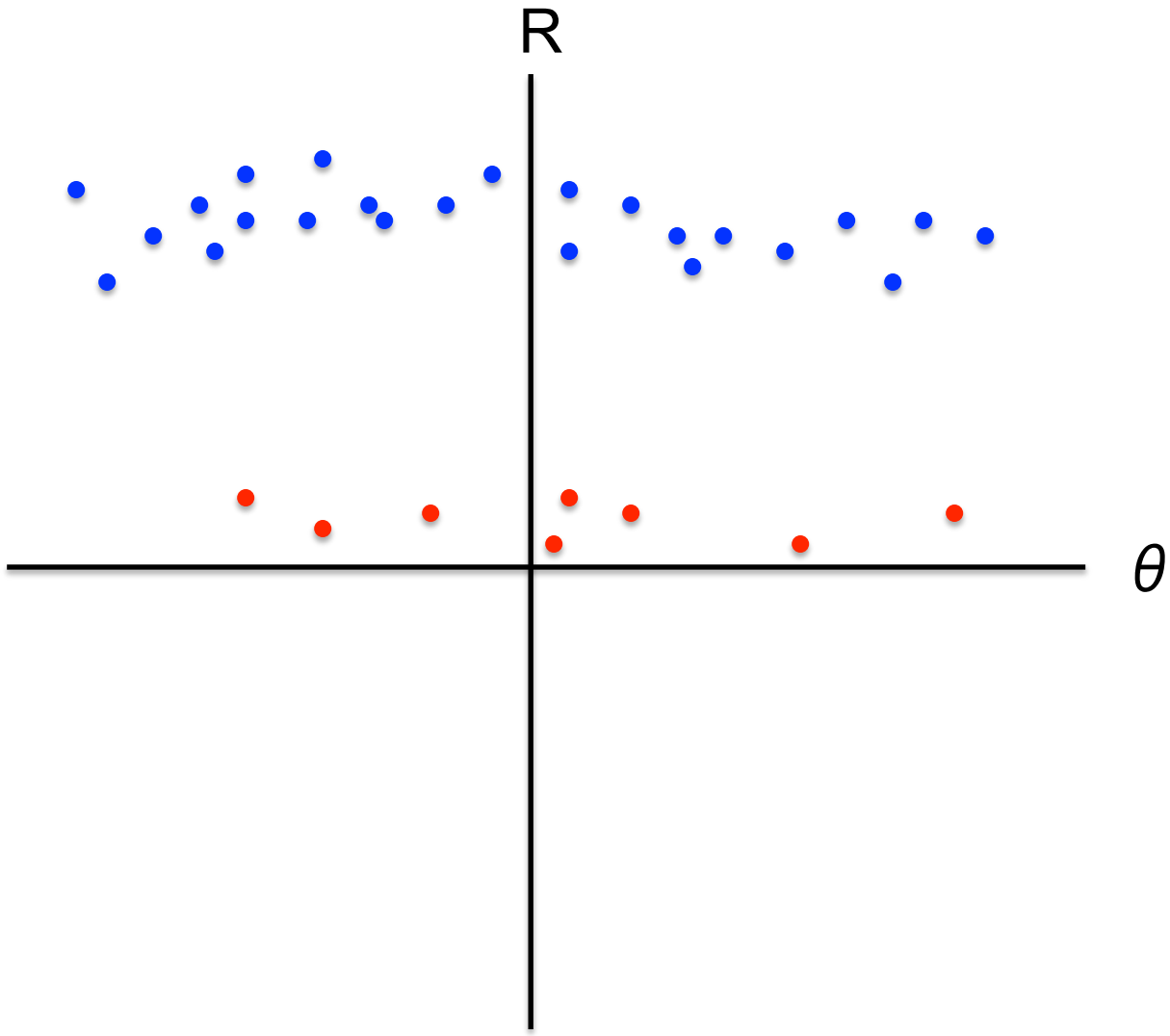




K-means not able to properly cluster

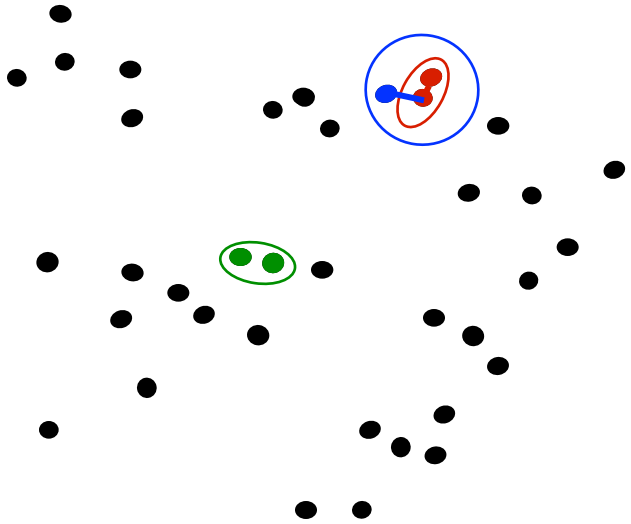


Changing the features (distance function) can help



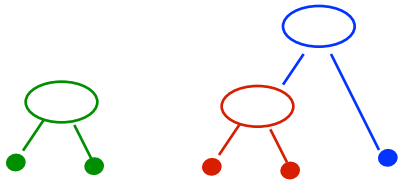
Agglomerative Clustering

- Agglomerative clustering:
  - First merge very similar instances
  - Incrementally build larger clusters out of smaller clusters



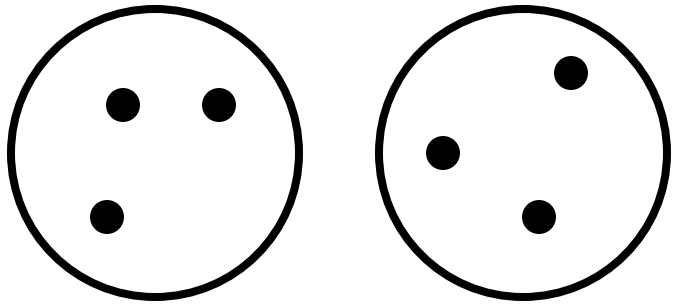
- Algorithm:
  - Maintain a set of clusters
  - Initially, each instance in its own cluster
  - Repeat:
    - Pick the two closest clusters
    - Merge them into a new cluster
    - Stop when there's only one cluster left

- Produces not one clustering, but a family of clusterings represented by a dendrogram



Agglomerative Clustering

- How should we define “closest” for clusters with multiple elements?

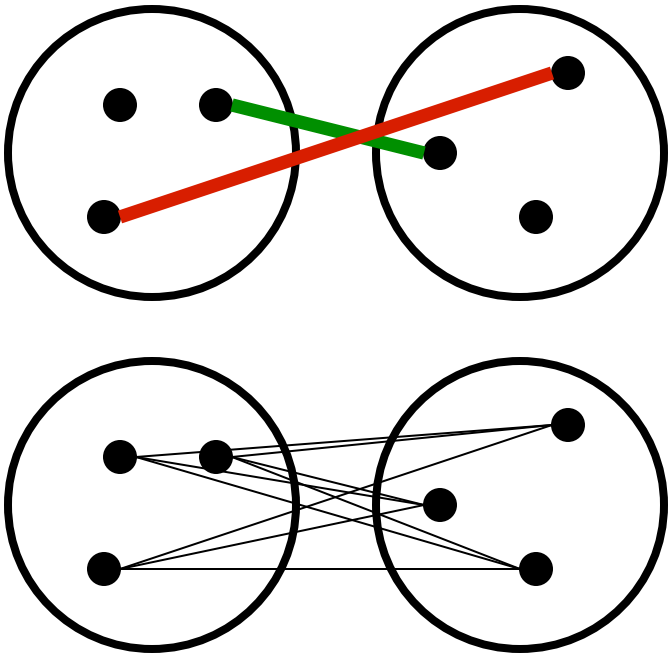


Agglomerative Clustering

- How should we define "closest" for clusters with multiple elements?

- Many options:
  - Closest pair
    (single-link clustering)
  - Farthest pair
    (complete-link clustering)
  - Average of all pairs

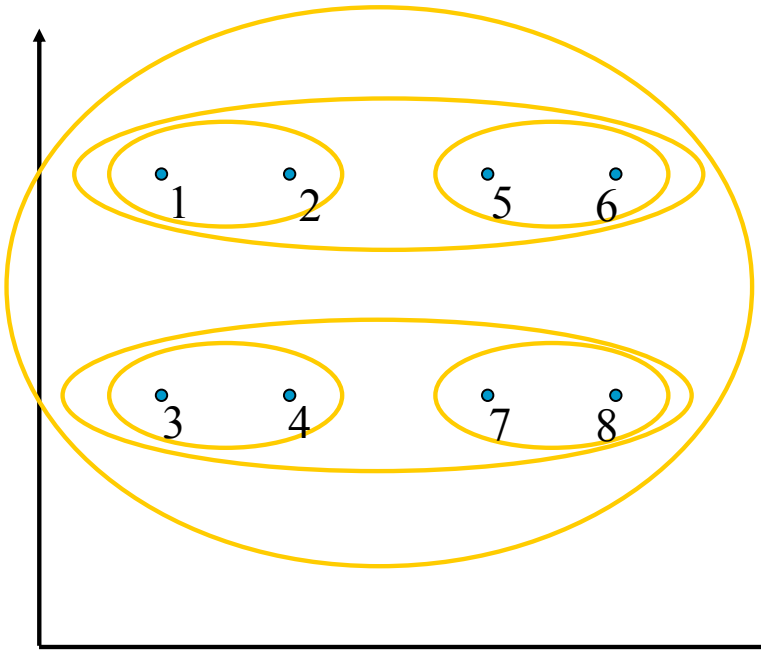
- Different choices create different clustering behaviors



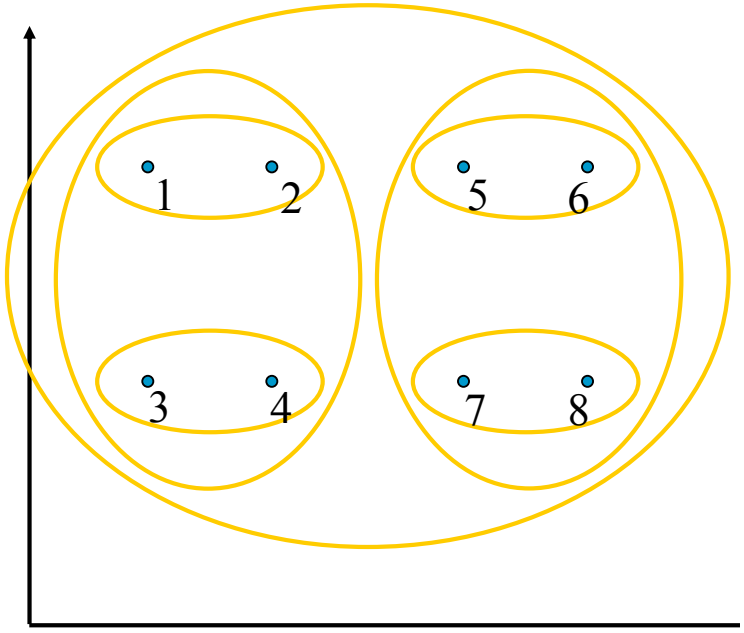
Agglomerative Clustering

- How should we define "closest" for clusters with multiple elements?

Closest pair
(single-link clustering)

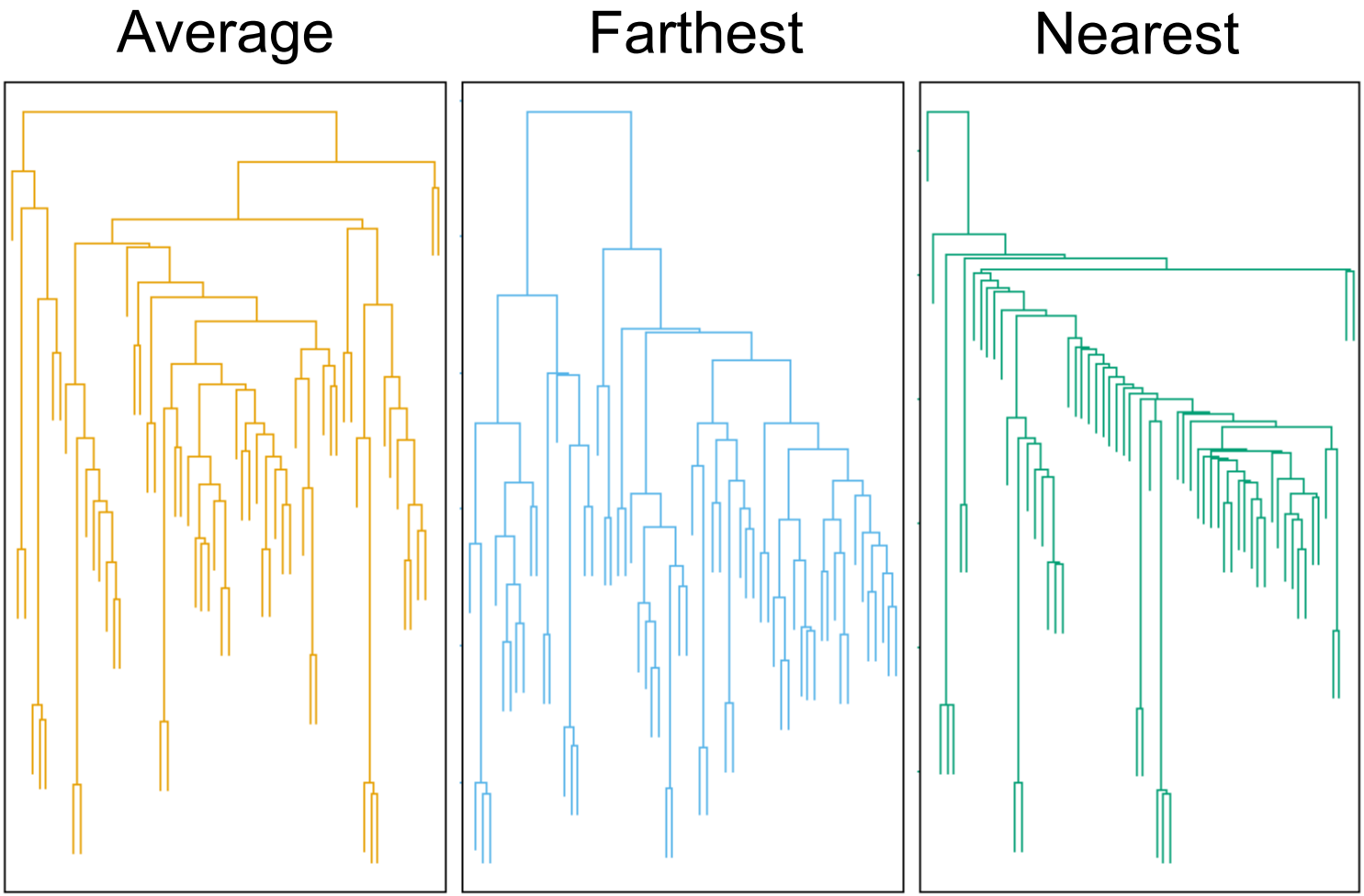


Farthest pair
(complete-link clustering)



[Pictures from Thorsten Joachims]

Clustering Behavior

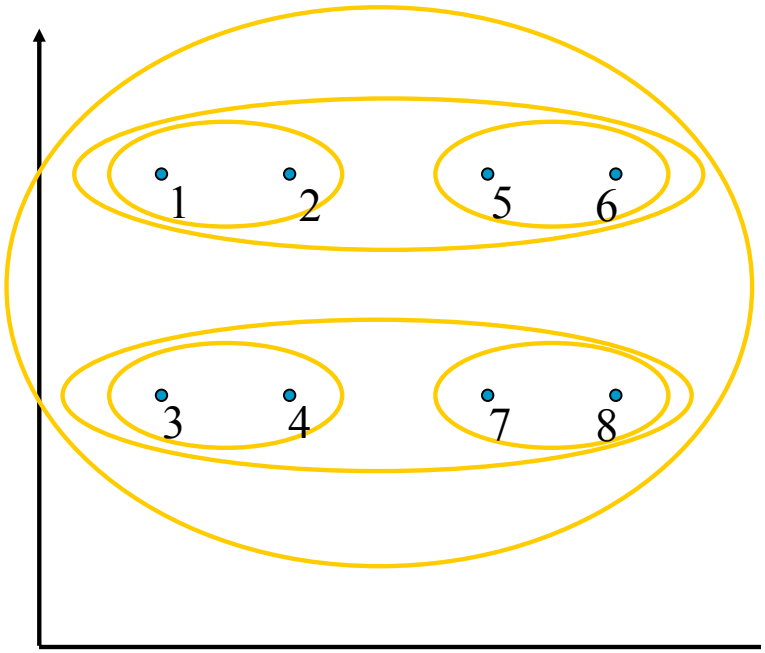


Mouse tumor data from [Hastie *et al.*]

Agglomerative Clustering

When can this be expected to work?

Closest pair
(single-link clustering)



Strong separation property:
All points are more similar to points in their own cluster than to any points in any other cluster

Then, the true clustering corresponds to some **pruning** of the tree obtained by single-link clustering!

Slightly weaker (stability) conditions are solved by average-link clustering

(Balcan et al., 2008)

Other cluster methods

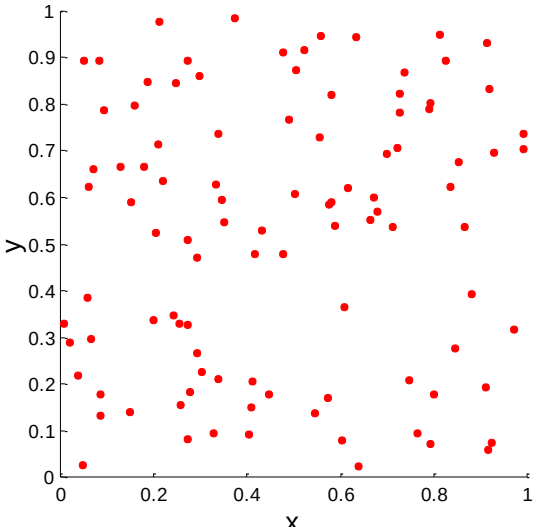
- DBSCAN
- Gaussian mixture model (GMM)
- Spectral clustering
- Biclustering
- Topic model
- Affinity propagation (Science-2007)
- DensityClust (Science-2014)

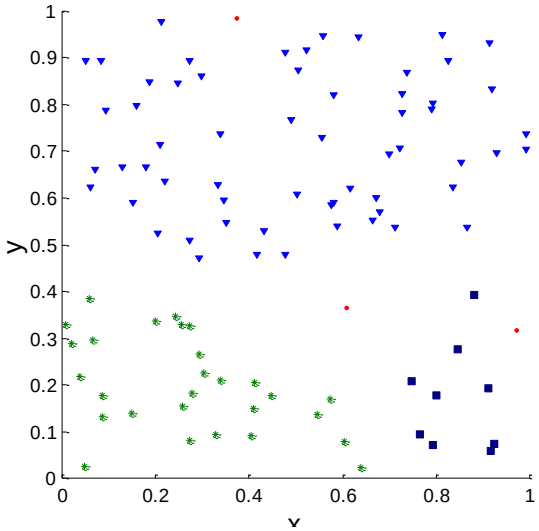
Cluster validation

- For supervised classification we have a variety of measures to evaluate how good our model is
  - Accuracy, precision, recall
- For cluster analysis, the analogous question is how to evaluate the “goodness” of the resulting clusters?
- But “clusters are in the eye of the beholder”!
- Then why do we want to evaluate them?
  - To avoid finding patterns in noise
  - To compare clustering algorithms
  - To compare two sets of clusters
  - To compare two clusters

Clusters found in random data

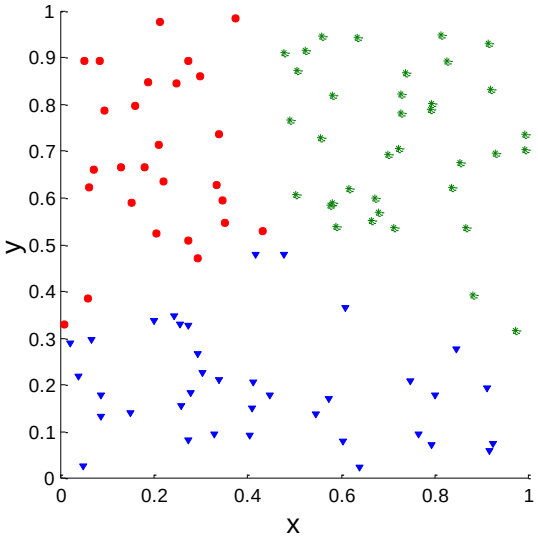
Random Points

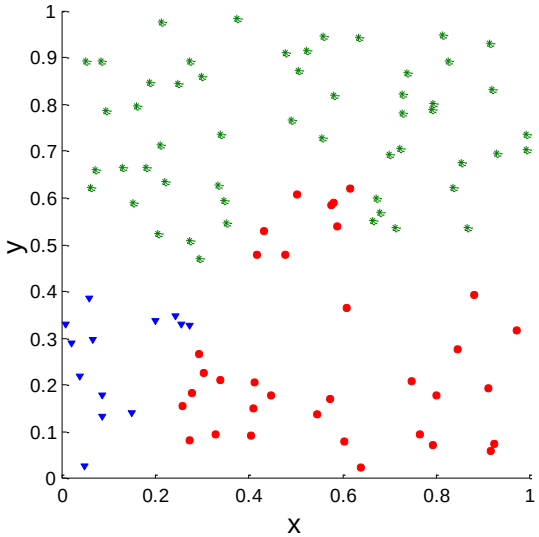




DBSCAN

K-means





Complete Link

Different aspects of cluster validation

- Determining the clustering tendency of a set of data, i.e., distinguishing whether non-random structure actually exists in the data.
- Comparing the results of a cluster analysis to externally known results, e.g., to externally given class labels.
- Evaluating how well the results of a cluster analysis fit the data without reference to external information
  - Use only the data
- Determining the ‘correct’ number of clusters.

Measures of cluster validity

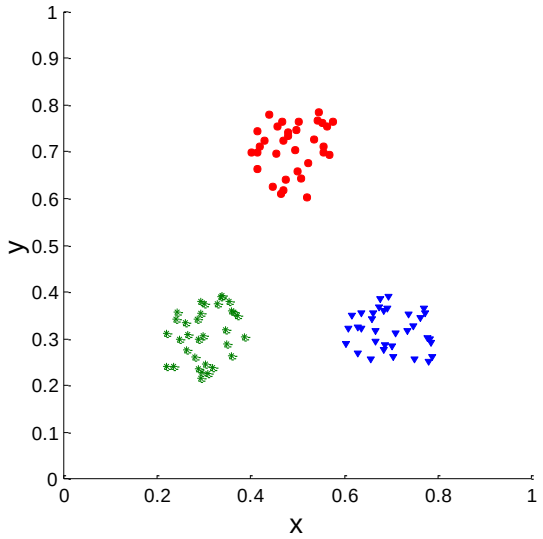
- Numerical measures that are applied to judge various aspects of cluster validity, are classified into the following three types.
  - External Index: Used to measure the extent to which cluster labels match externally supplied class labels.
    - Entropy
  - Internal Index: Used to measure the goodness of a clustering structure without respect to external information.
    - Sum of Squared Error (SSE)
  - Relative Index: Used to compare two different clusterings or clusters.
    - Often an external or internal index is used for this function, e.g., SSE or entropy
- Sometimes these are referred to as criteria instead of indices.
  - However, sometimes criterion is the general strategy and index is the numerical measure that implements the criterion.

Measures cluster validity via correlation

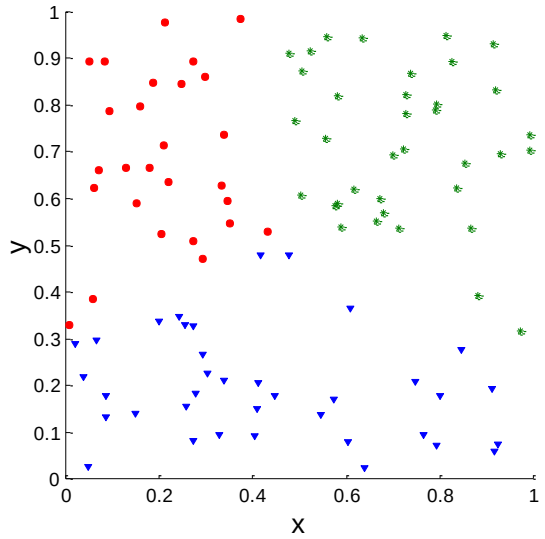
- Two matrices
  - Proximity matrix
  - “Incidence” matrix
    - One row and one column for each data point
    - An entry is 1 if the associated pair of points belong to the same cluster
    - An entry is 0 if the associated pair of points belong to different clusters
  - Computer the correlation between the two matrices
    - Since the matrices are symmetric, only the correlation between n(n-1)/2 entries needs to be calculated
- High correlation indicates that points that belong to the same cluster are close to each other.
- Not a good measure for some density or continuity based clusters

Measures cluster validity via correlation

- Correlation of incidence and proximity matrices for the K-means clusterings of the following two datasets



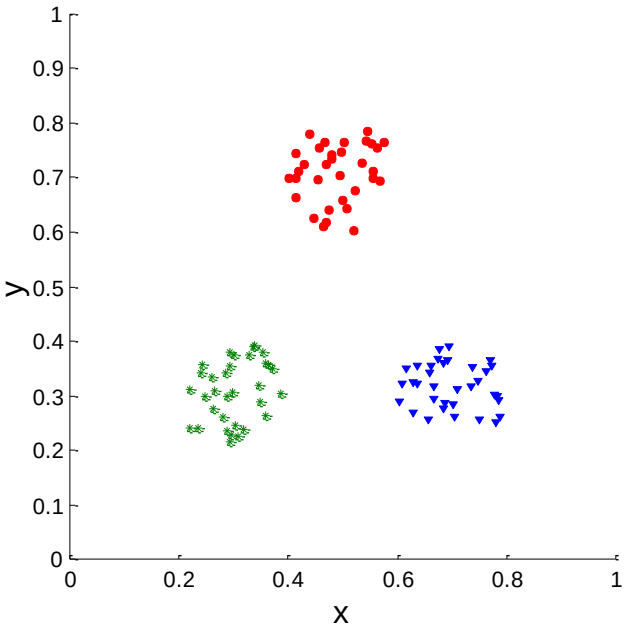
Corr = -0.9235

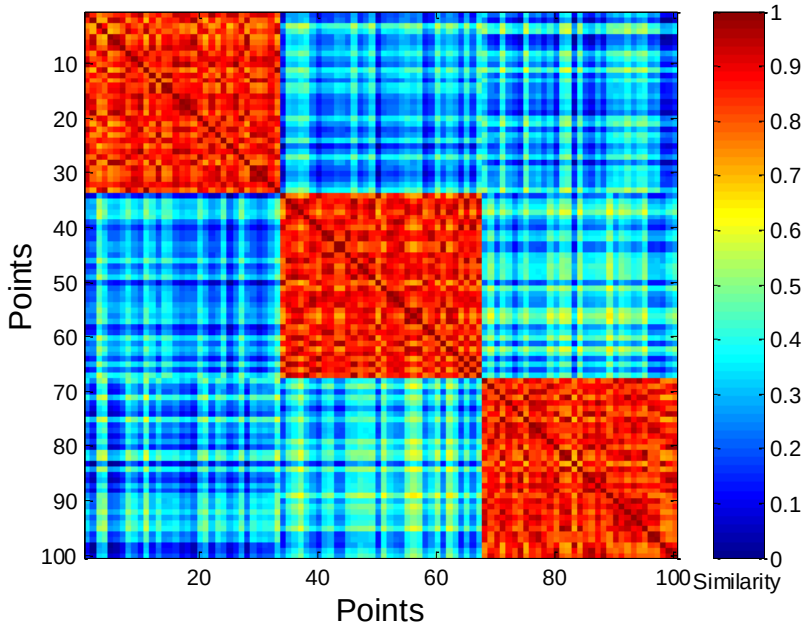


Corr = -0.5810

Using similarity matrix for cluster validation

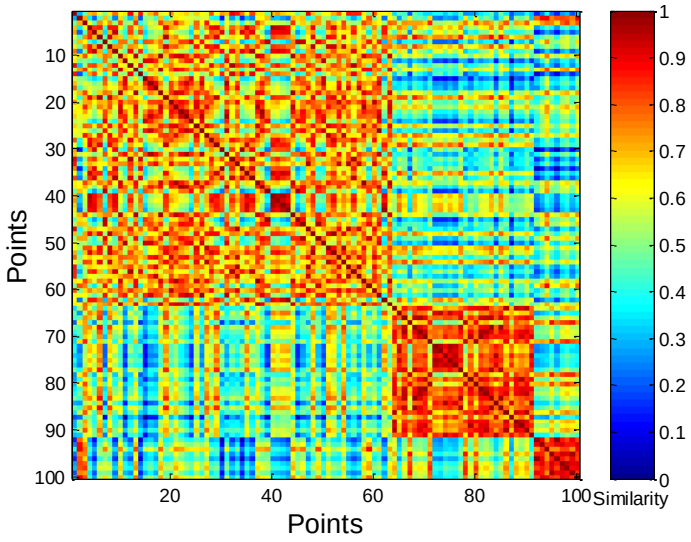
- Order the similarity matrix with respect to cluster labels and inspect visually

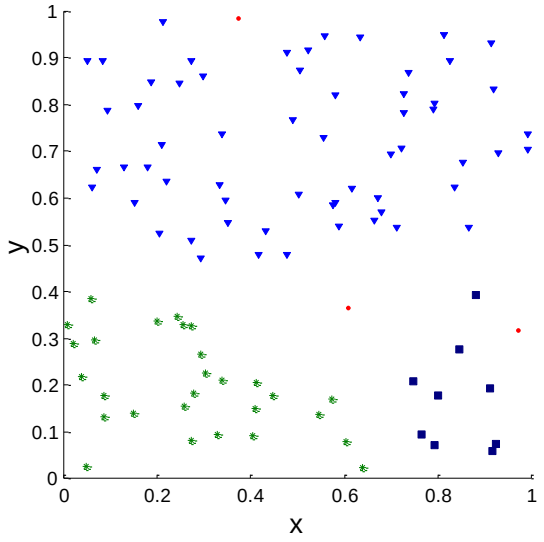




Using similarity matrix for cluster validation

- Clusters in random data are not so crisp

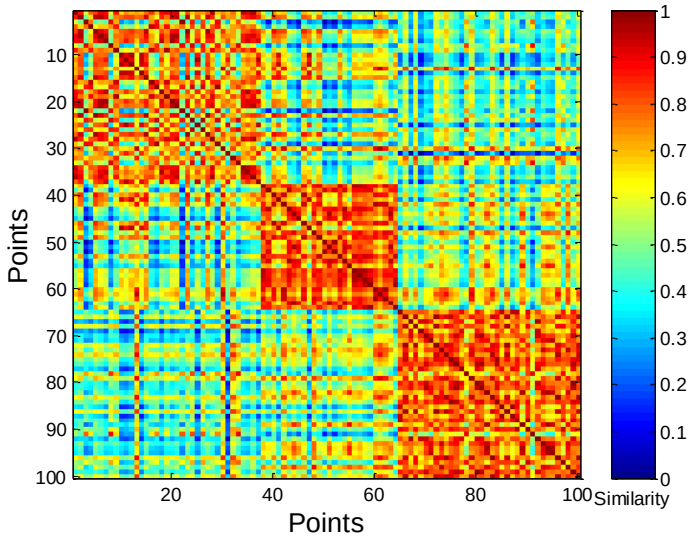


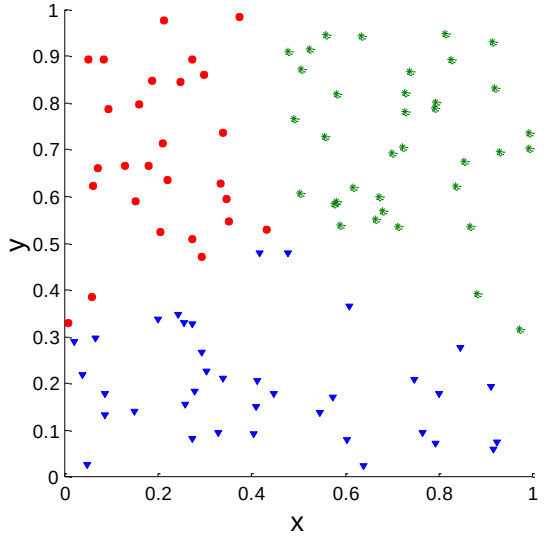


DBSCAN

Using similarity matrix for cluster validation

- Clusters in random data are not so crisp

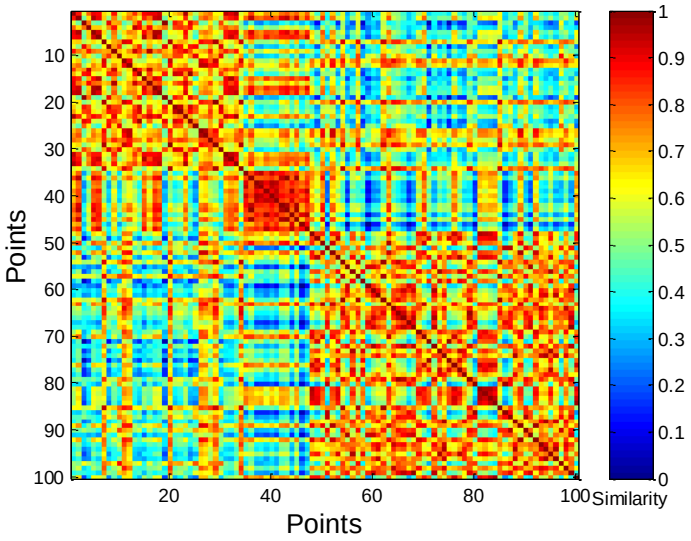


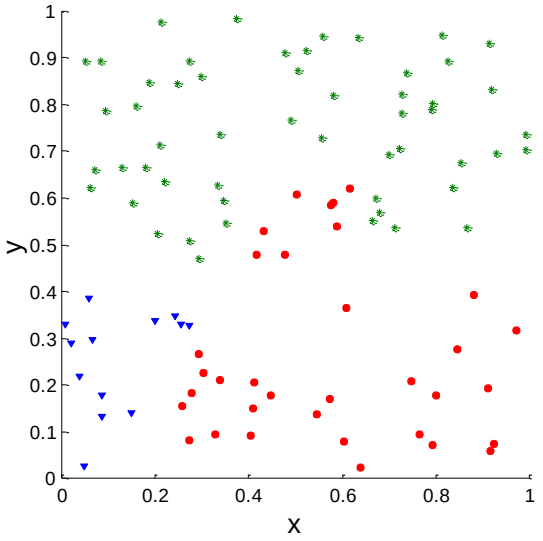


K-means

Using similarity matrix for cluster validation

- Clusters in random data are not so crisp

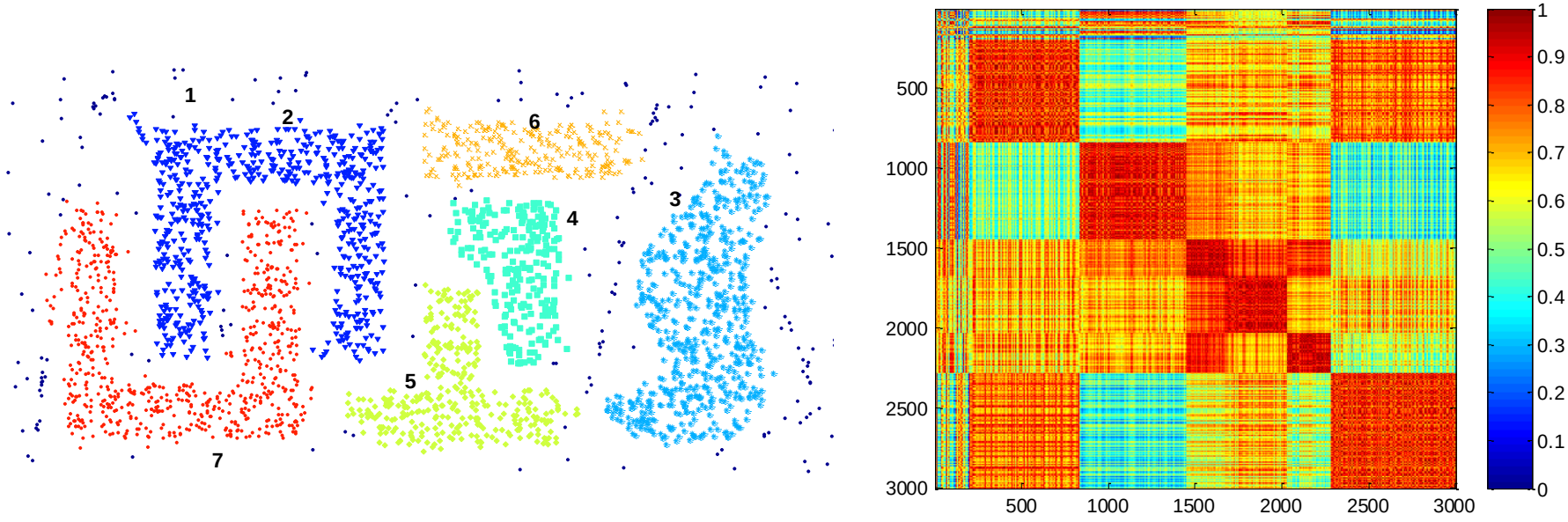




Complete Link

Using similarity matrix for cluster validation

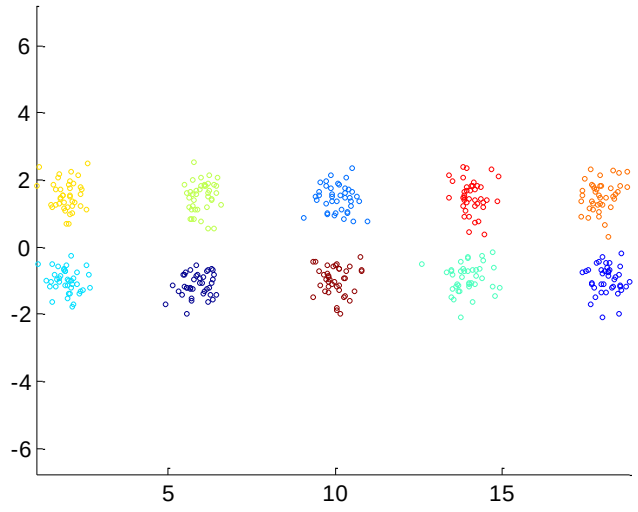
- Clusters in random data are not so crisp

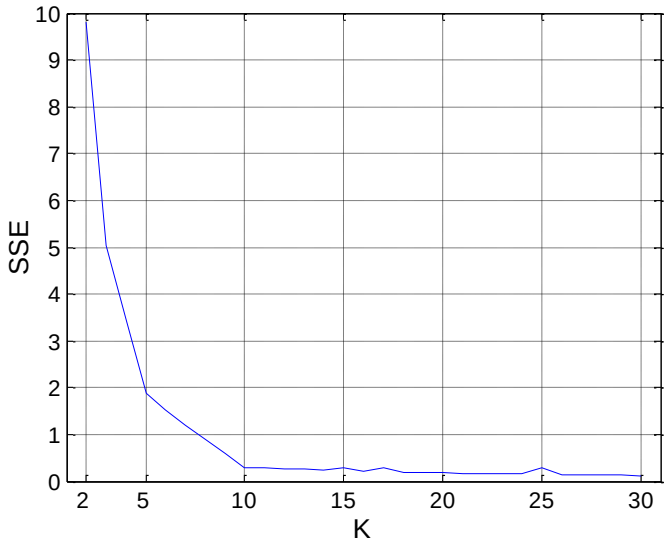


DBSCAN

Internal Measures: SSE

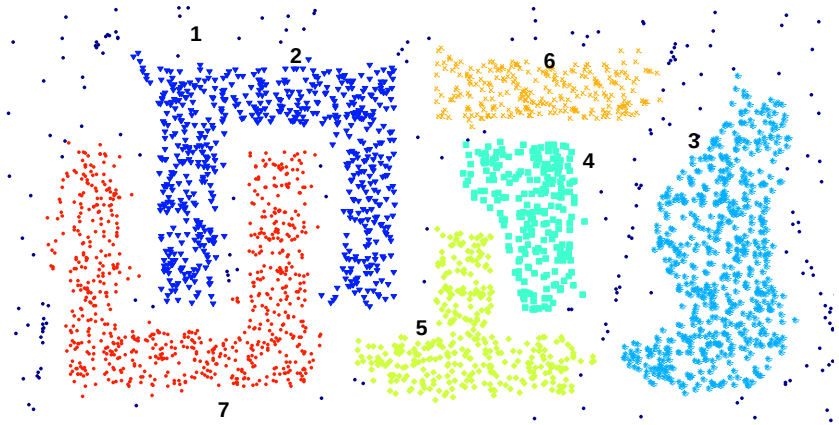
- Clusters in more complicated figures aren't well separated
- Internal Index: Used to measure the goodness of a clustering structure without respect to external information
  - SSE
- SSE is good for comparing two clusterings or two clusters (average SSE).
- Can also be used to estimate the number of clusters

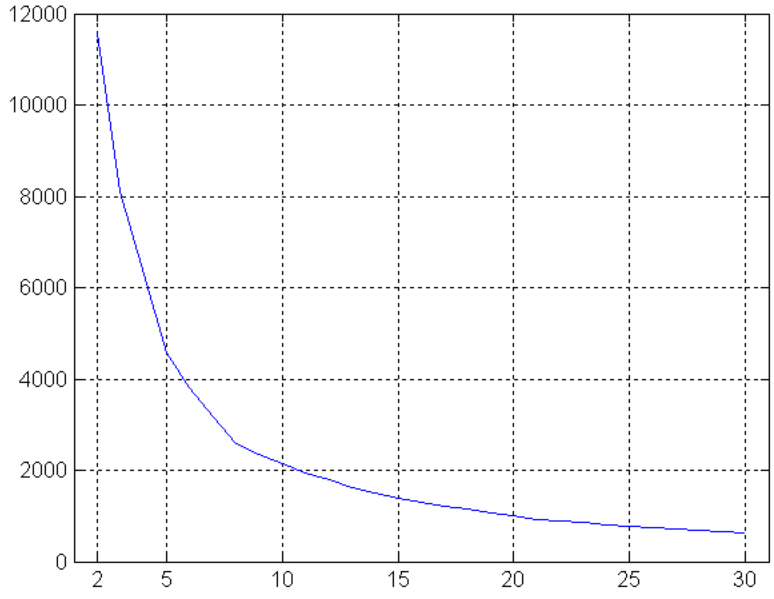




Using similarity matrix for cluster validation

- SSE curve for a more complicated data set





SSE of clusters found using K-means

Final Comment on Cluster Validity

"The validation of clustering structures is the most difficult and frustrating part of cluster analysis.

Without a strong effort in this direction, cluster analysis will remain a black art accessible only to those true believers who have experience and great courage."

Algorithms for Clustering Data, Jain and Dubes