2011 Clustering in Machine Learning

Motivation: Why Clustering?

Problem: Identify (a small number of) groups of similar objects in a given (large) set of object.

Goals:

- Find representatives for homogeneous groups →**Data Compression**
- Find "natural" clusters and describe their properties →**"natural" Data Types**
- Find suitable and useful grouping →**"useful" Data Classes**
- Find unusual data object →**Outlier Detection**

Examples of Clustering Applications

- Plant/Animal Classification
- Book Ordering
- Cloth Sizes
- Fraud Detection (Find outlier)

Major Clustering Approaches

- Partitioning algorithms/Representative-based/Prototype-based Clustering Algorithm: Construct and search various partitions and then evaluate them by some criterion or fitness function →Kmeans
- Hierarchical algorithms: Create a hierarchical decomposition of the set of data (or objects) using some criterion
- Density-based: based on connectivity and density functions →DBSCAN, DENCLUE,…
- Grid-based: based on a multiple-level granularity structure
- Graph-based: constructs a graph and then clusters the graph →SNN
- Model-based: A model is hypothesized for each of the clusters and the idea is to find the best fit of that model to each other →EM

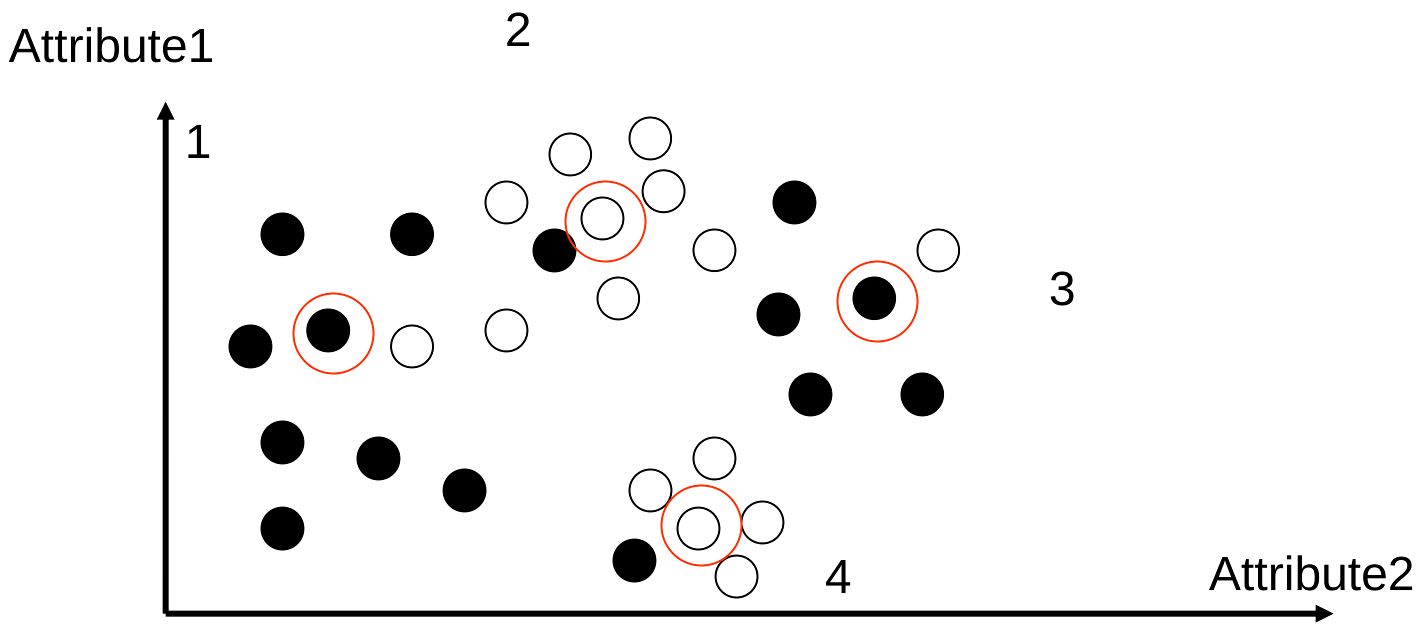
Representative-Based Clustering

- Aims at finding a set of objects among all objects (called **representatives**) in the data set that best represent the objects in the data set. Each representative corresponds to a cluster.
- The remaining objects in the data set are then clustered around these *representatives* by assigning objects to the cluster of the closest representative.

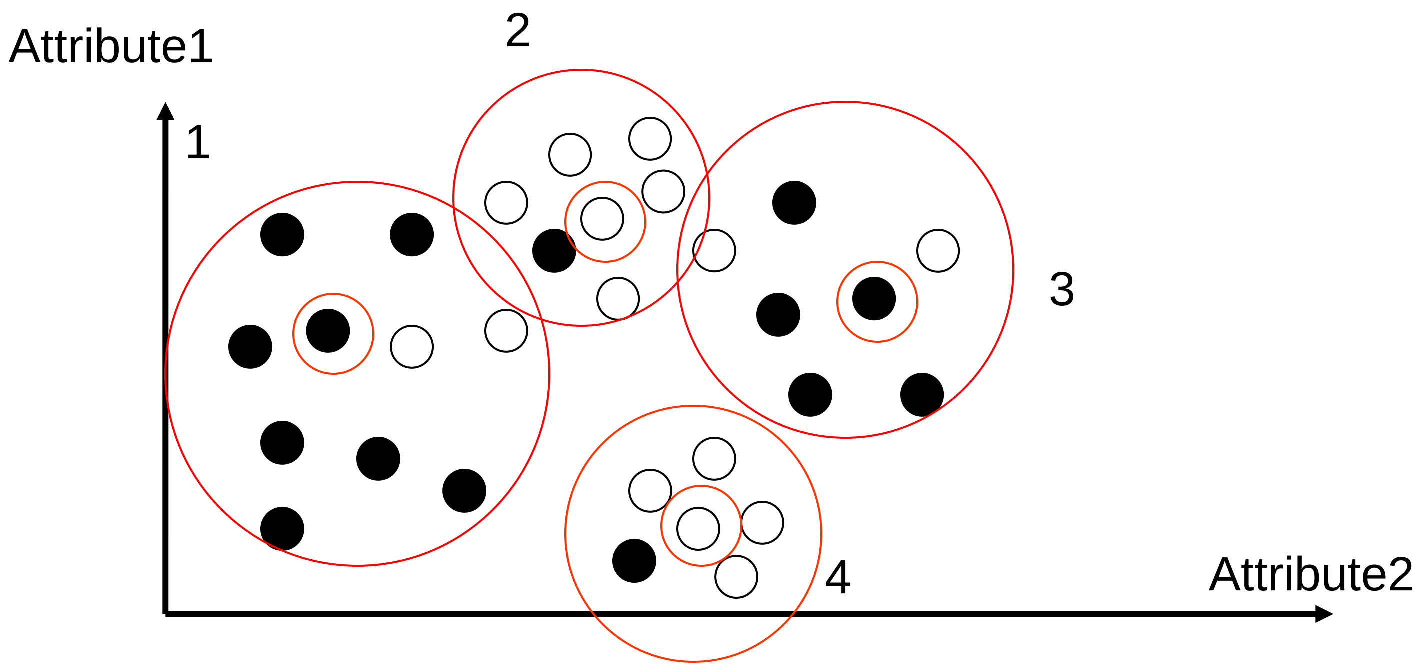
Remarks:

1. The popular *k-medoid algorithm*, also called *PAM*, is a representative-based clustering algorithm; K-means also shares the characteristics of representative-based clustering, except that the representatives used by k-means not necessarily have to belong to the data set.
2. If the representative do not need to belong to the dataset we call the algorithms prototype-based clustering. K-means is a **prototype-based** clustering algorithm

Representative-Based Clustering … (Continued)



Representative-Based Supervised Clustering … (continued)



Objective of RSC: Find a subset O_R of O such that the clustering X obtained by using the objects in O_R as representatives minimizes q(X); q is an objective/fitness function.

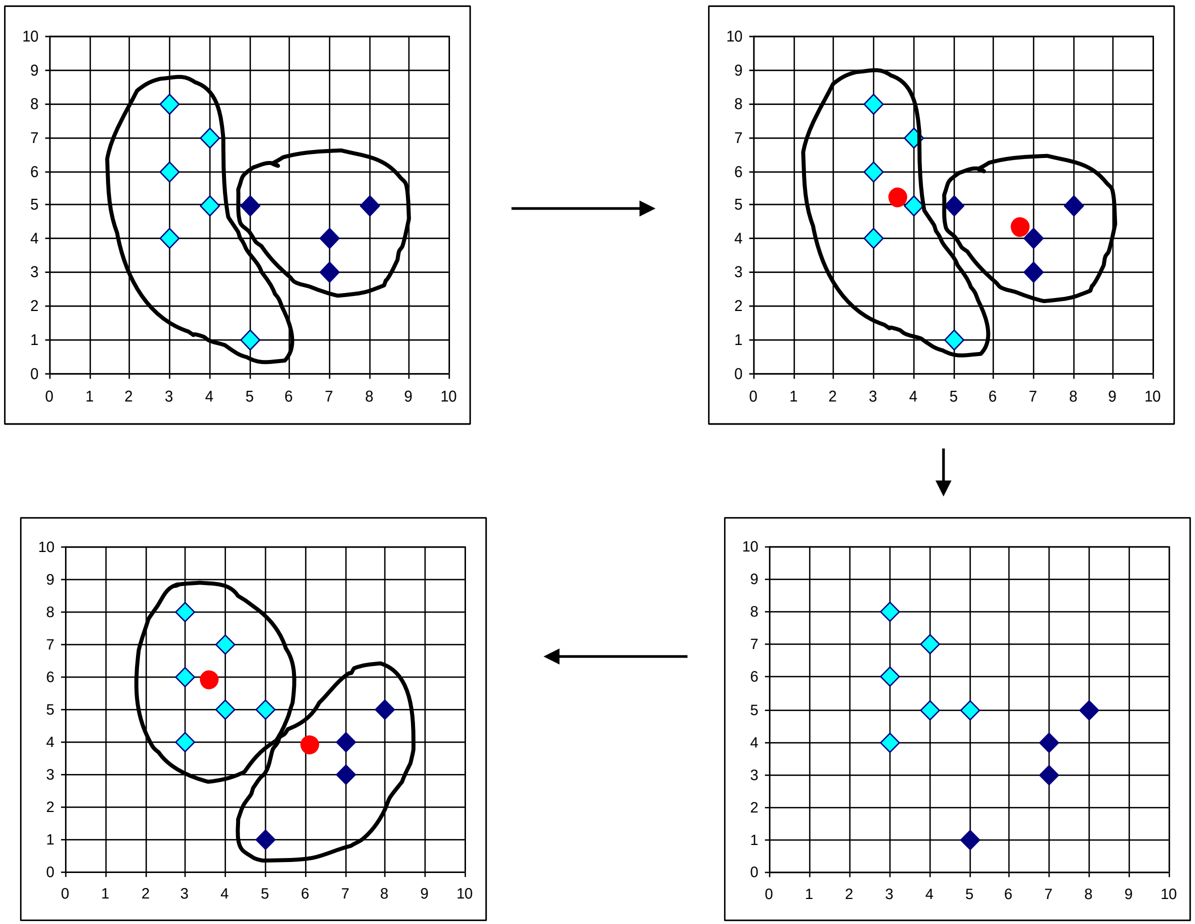
The *K-Means* Clustering Method

- Given *k*, the *k-means* algorithm is implemented in 4 steps:
  1. Partition objects into *k* nonempty subsets
  2. Compute seed points as the centroids of the clusters of the current partition. The centroid is the center (mean point) of the cluster.
  3. Assign each object to the cluster with the nearest seed point.
  4. Go back to Step 2, stop when no more new assignment.

The *K-Means* Clustering Method

- Example

Cluster→"New" Model



Model→"New" Cluster

Comments on *K-Means*

Strength

- *Relatively efficient*: *O*(*t*k*n*d*), where *n* is # objects, *k* is # clusters, and *t* is # iterations, d is the # dimensions. Usually, d, *k*, *t* << *n*; in this case, K-Mean's runtime is O(n).
- Storage only O(n)—in contrast to other representative-based algorithms, only computes distances between centroids and objects in the dataset, and not between objects in the dataset; therefore, the distance matrix does not need to be stored.
- Easy to use; well studied; we know what to expect
- Finds l*ocal optimum of the SSE fitness function*. The *global optimum* may be found using techniques such as: *deterministic annealing* and *genetic algorithms*
- Implicitly uses a fitness function (finds a local minimum for SSE see later) --- does not waste time computing fitness values

Weakness

- Applicable only when *mean* is defined --- what about categorical data?
- Need to specify *k,* the *number* of clusters, in advance
- Sensitive to *outliers*
- Not suitable to discover clusters with non-convex shapes
- Sensitive to initialization; bad initialization might lead to bad results.

Complication: Empty Clusters

K=3

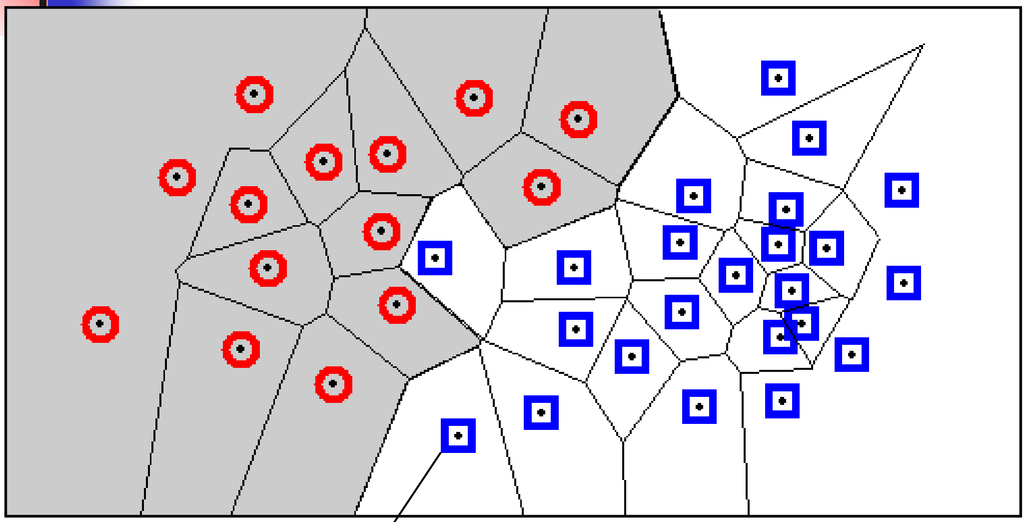
X X　　　　　　　　　X X
　X　　　　　　　　　　X
X X　　　　　　　　　X X

We assume that the k-means initialization assigns the green, blue, and brown points to a single cluster; after centroids are computed and objects are reassigned, it can easily be seen that that the brown cluster becomes empty.

Convex Shape Cluster

- Convex Shape: if we take two points belonging to a cluster then all the points on a direct line connecting these two points must also in the cluster.
- Shape of K-means/K-mediods clusters are convex polygons$\subseteq$ Convex Shape.
- Shapes of clusters of a representative-based clustering algorithm can be computed as a Voronoi diagram for the set of cluster representatives.
- Voronoi cells are always convex, but there are convex shapes that a different from those of Voronoi cells.

Voronoi Diagram for a Representative-based Clustering



Each cell contains one representatives, and every location within the cell is closer to that sample than to any other sample.

A **Voronoi diagram** divides the space into such cells.

Voronoi cells define cluster boundary!

Cluster Representative (e.g. medoid/centroid)

EM — Expectation Maximization

- EM — A popular iterative refinement algorithm
- Uses k-Gaussians; one for each cluster
- An extension to k-means
  - Assign each object to a cluster according to a weight (prob. distribution)
  - New means/covariances are computed based on weighted measures
- General idea
  - Starts with an initial estimate of the parameter vector
  - Iteratively rescores the patterns against the mixture density produced by the parameter vector
  - The rescored patterns are used to update the parameter updates
  - Patterns belonging to the same cluster, if they are placed by their scores in a particular component
- Algorithm converges fast but may not be in global optima

The EM (Expectation Maximization) Algorithm

- Initially, randomly assign k cluster centers
- Iteratively refine the clusters based on two steps
  - Expectation step: assign each data point X_i to cluster C_i with the

$$P(X_i \in C_k) = p(C_k|X_i) = \frac{p(C_k)p(X_i|C_k)}{p(X_i)},$$

  - Maximization step:
    - Estimation of model parameters

$$m_k = \frac{1}{N}\Sigma_{i=1}^{N}\frac{X_i P(X_i \in C_k)}{\Sigma_j P(X_i \in C_j)}.$$