CLUSTERING Methods

Prof. Sukhendu Das
Deptt. of CS&E,
IIT Madras,
Chennai, INDIA.

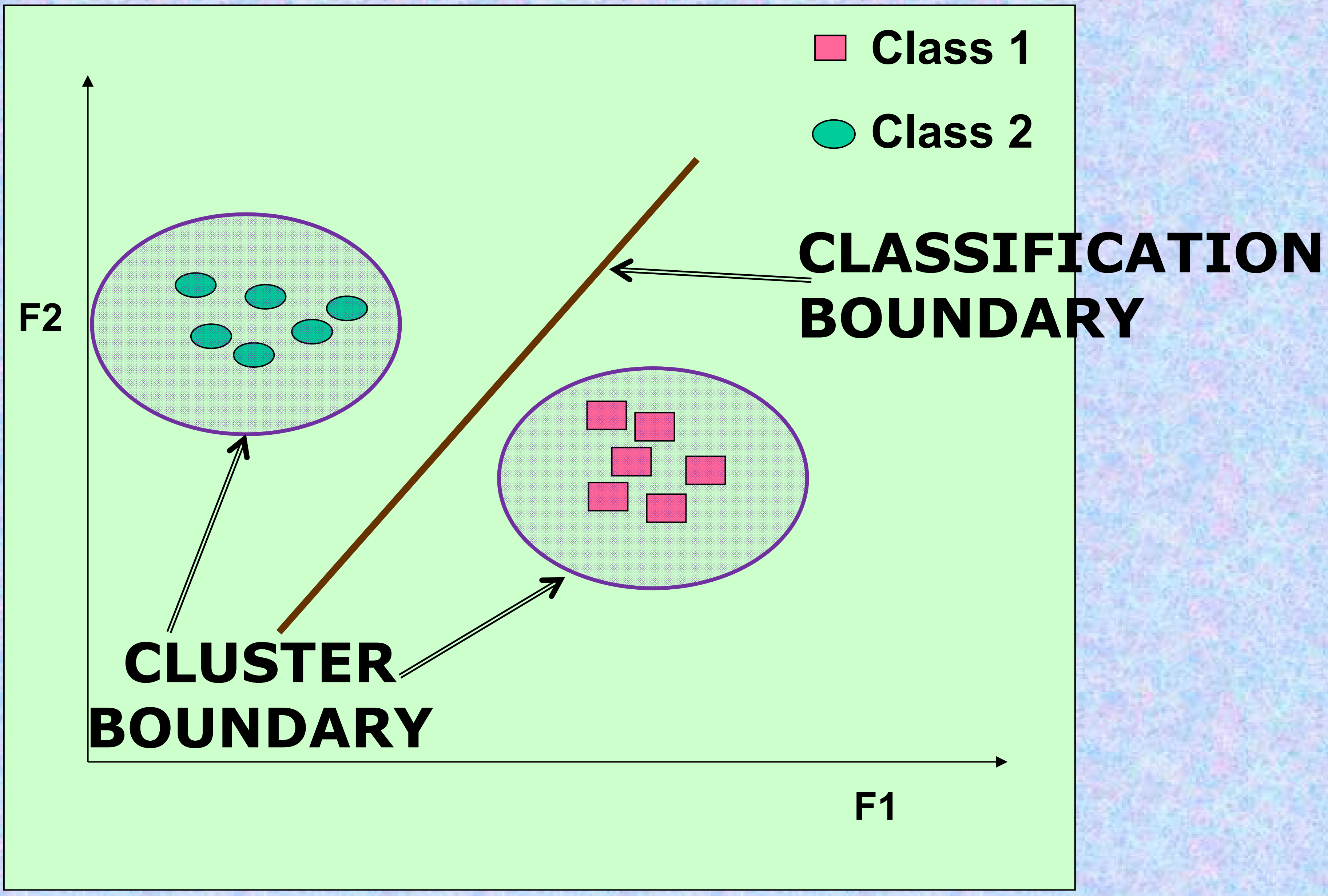
Email: sdas@cse.iitm.ac.in

What is Cluster Analysis?

- Cluster: A collection of data objects
  - similar (or related) to one another within the same group
  - dissimilar (or unrelated) to the objects in other groups
- Cluster analysis (or *clustering*, *data segmentation, …*)
  - Finding similarities between data according to the characteristics found in the data and grouping similar data objects into clusters
- Unsupervised learning: no predefined classes (i.e., *learning by observations* vs. learning by examples: supervised)
- Typical applications
  - As a stand-alone tool to get insight into data distribution
  - As a preprocessing step for other algorithms

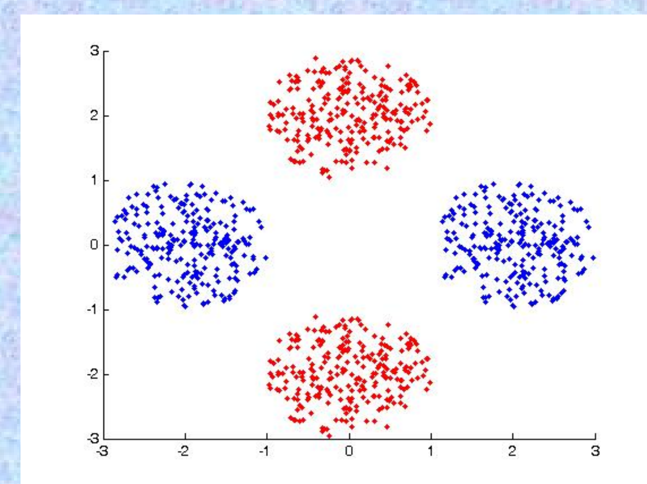
Clustering: Application Examples

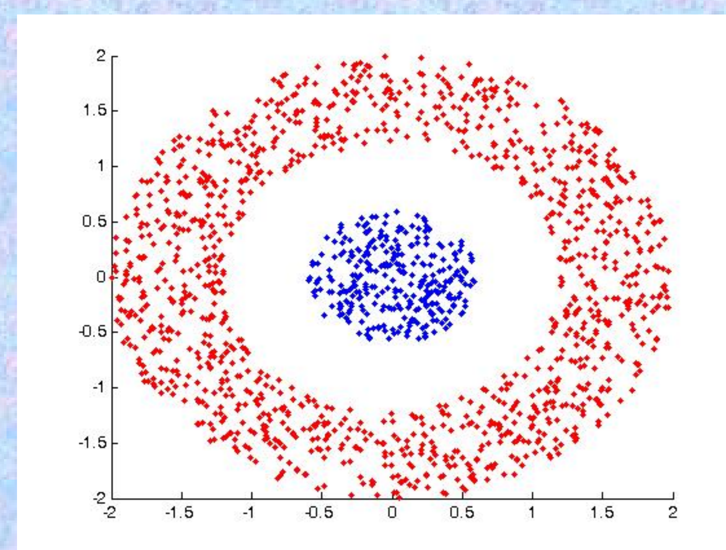
- **Biology**: taxonomy of living things: kingdom, phylum, class, order, family, genus and species
- **Information retrieval**: document clustering
- **Land use**: Identification of areas of similar land use in an earth observation database
- **Marketing**: Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs
- **City-planning**: Identifying groups of houses according to their house type, value, and geographical location
- **Earth-quake studies**: Observed earth quake epicenters should be clustered along continent faults
- **Climate**: understanding earth climate, find patterns of atmospheric and ocean
- **Economic Science**: market research

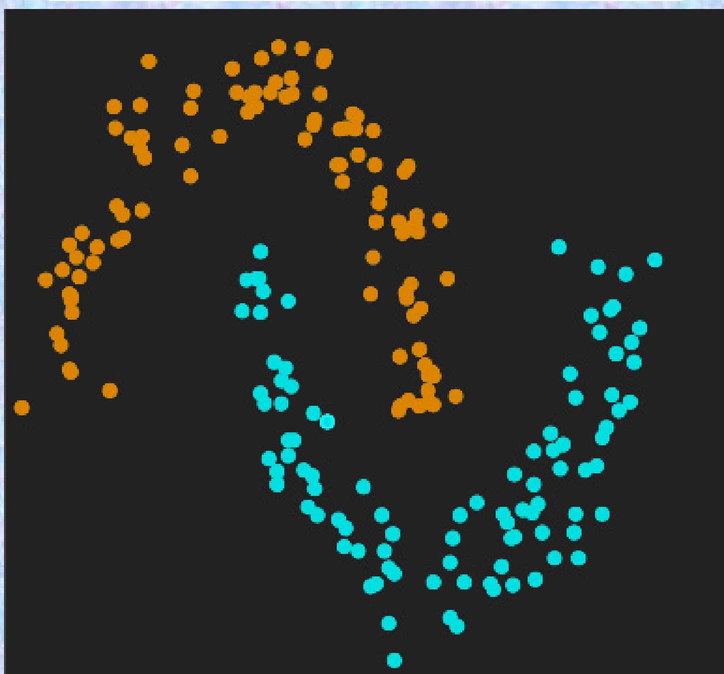


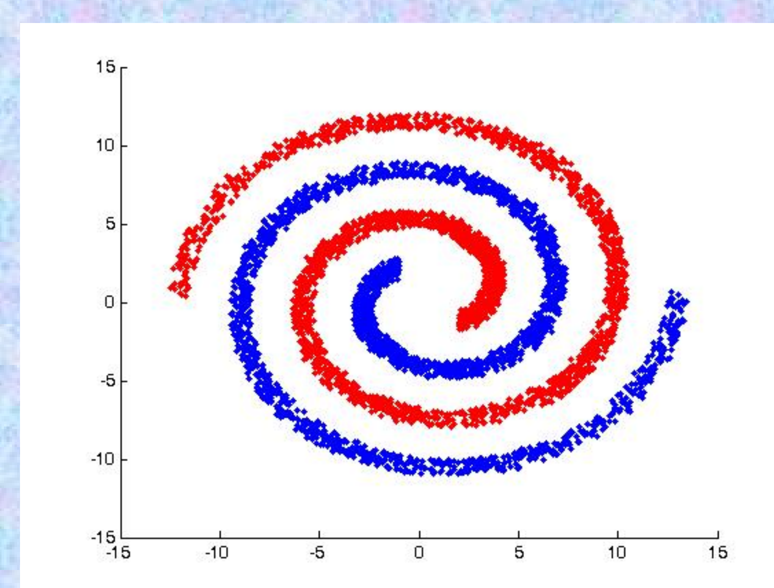
Sample points in a two-dimensional feature space

Complex cases of classification and clustering









CLUSTERING	CLASSIFICATION
Data Points have no labels	Most data points have labels

METHODS OF

CLUSTERING AND CLASSIFICATION

- REPRESENTATIVE POINTS
- Split & MERGE
- LINKAGE
- SOM
- MODEL-BASED
- VECTOR QUANTIZATION

Quality: What Is Good Clustering?

- A good clustering method will produce high quality clusters
  - high intra-class similarity: cohesive within clusters
  - low inter-class similarity: distinctive between clusters
- The quality of a clustering method depends on
  - the similarity measure used by the method
  - its implementation, and
  - Its ability to discover some or all of the hidden patterns

Considerations for Cluster Analysis

- Partitioning criteria
  - Single level vs. hierarchical partitioning (often, multi-level hierarchical partitioning is desirable)
- Separation of clusters
  - Exclusive (e.g., one customer belongs to only one region) vs. non-exclusive (e.g., one document may belong to more than one class)
- Similarity measure
  - Distance-based (e.g., Euclidian, road network, vector) vs. connectivity-based (e.g., density or contiguity)
- Clustering space
  - Full space (often when low dimensional) vs. subspaces (often in high-dimensional clustering)

Major Clustering Approaches (I)

- **Partitioning approach:**
  - **Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of square errors**
  - **Typical methods: k-means, k-medoids, CLARANS**
- **Hierarchical approach:**
  - **Create a hierarchical decomposition of the set of data (or objects) using some criterion**
  - **Typical methods: Diana, Agnes, BIRCH, CAMELEON**
- **Density-based approach:**
  - **Based on connectivity and density functions**
  - **Typical methods: DBSCAN, OPTICS, DenClue**
- **Grid-based approach:**
  - **based on a multiple-level granularity structure**
  - **Typical methods: STING, WaveCluster, CLIQUE**

Major Clustering Approaches (II)

- **Model-based:**
  - **A model is hypothesized for each of the clusters and tries to find the best fit of that model to each other**
  - **Typical methods: EM, SOM, COBWEB**
- **Frequent pattern-based:**
  - **Based on the analysis of frequent patterns**
  - **Typical methods: p-Cluster**
- **User-guided or constraint-based:**
  - **Clustering by considering user-specified or application-specific constraints**
  - **Typical methods: COD (obstacles), constrained clustering**
- **Link-based clustering:**
  - **Objects are often linked together in various ways**
  - **Massive links can be used to cluster objects: SimRank, LinkClus**

GENERAL CATEGORIES of CLUSTERING DATA

- **Hierarchical (linkage based)**
  - **Agglomerative**
  - **Divisive**
- **Partitional**
  - **Exclusive**
    - MST
    - K-mean
    - K-medoid
  - **Probabilistic**
    - GMM
    - FCM

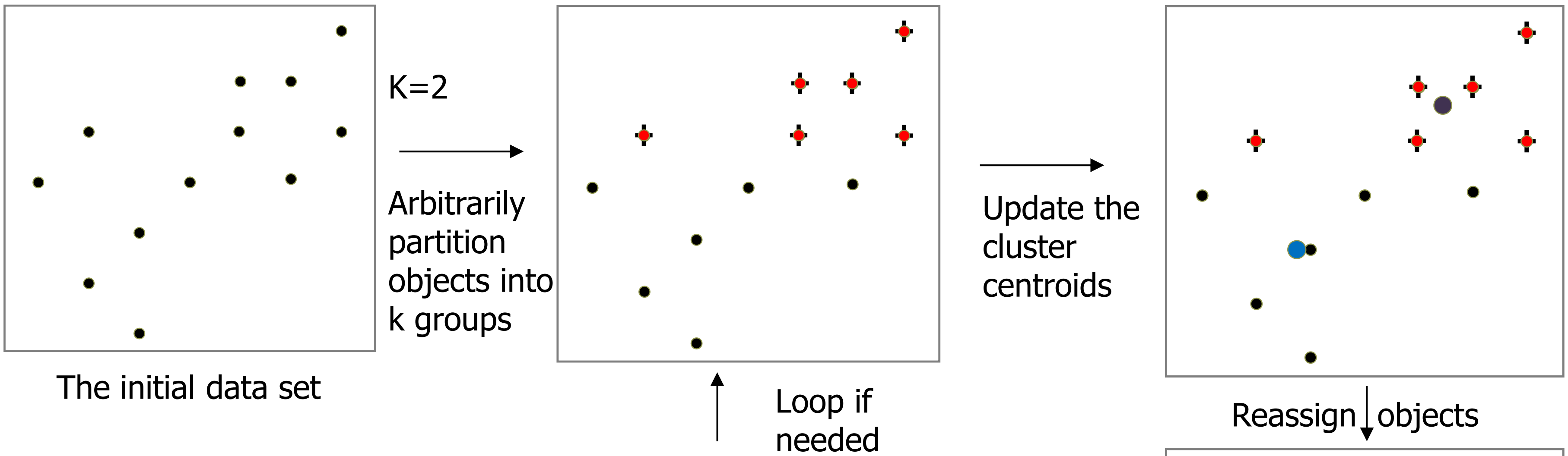
Alternative view of
Algorithms for CLUSTERING

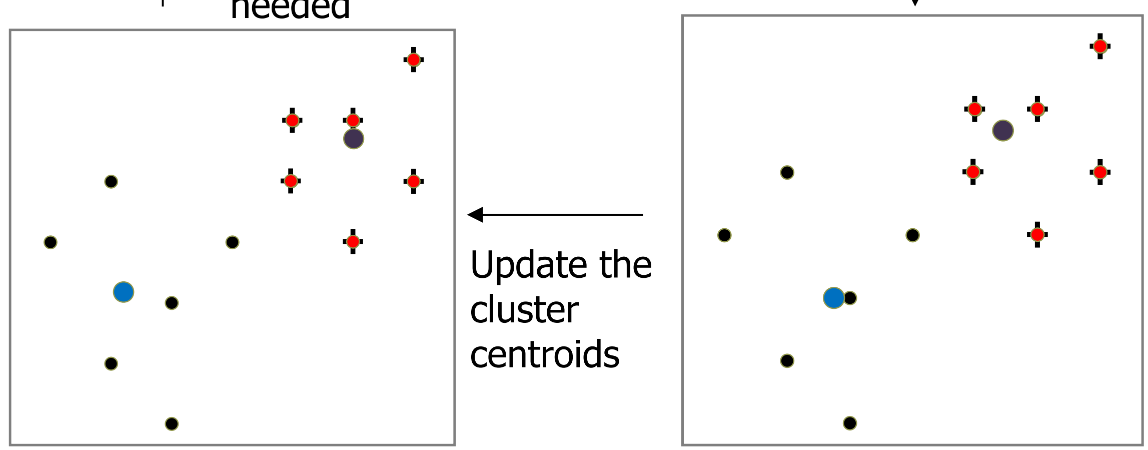
- Unupervised Learning/Classification:
  - K-means; K-medoid

- Density Estimation :
  - (i) Parametric
    - Gaussian
    - MOG (Mixture of Gaussians)
    - Dirichlet, Beta etc.
    - Branch and Bound Procedure
    - Piecewise Quadratic Boundary
    - Nearest Mean Classifier
    - MLE (maximum Likelihood Estimate)

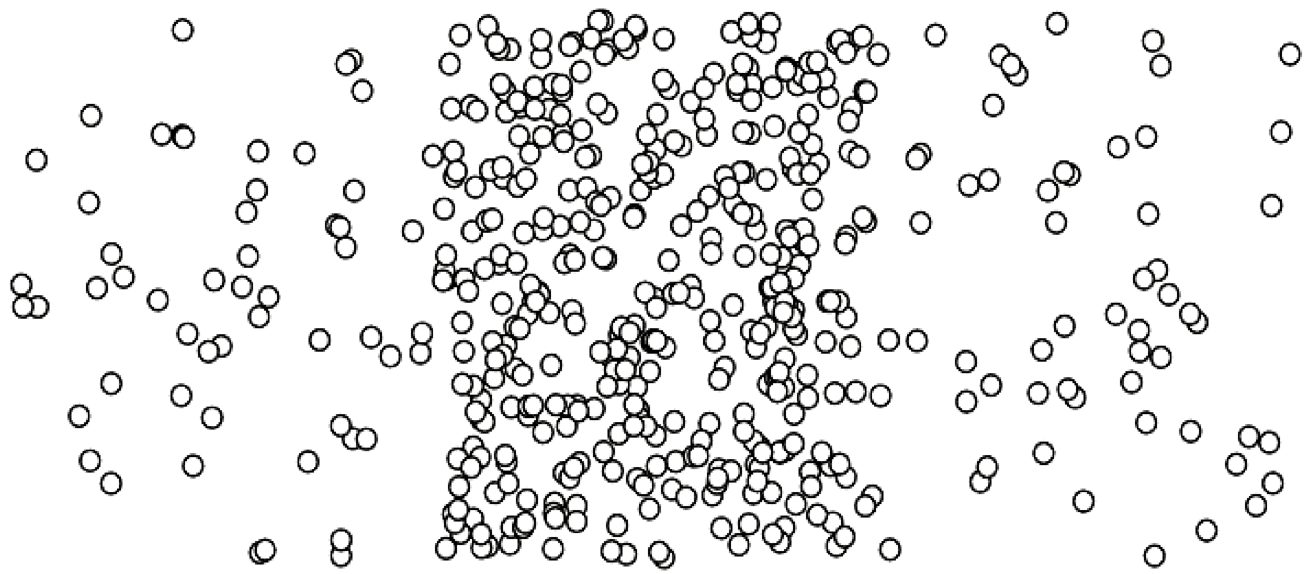
- **Density Estimation :**
  - **(ii) Non-Parametric**
    - **Histogram**
    - **Neighborhood**
    - **Kernel Methods**
    - **Graph Theoretic**
    - **Iterative Valley Seeking**

An Example of *K-Means* Clustering





- Partition objects into *k* nonempty subsets
- Repeat
  - Compute centroid (i.e., mean point) for each partition
  - Assign each object to the cluster of its nearest centroid
- Until no change



FCM - Fuzzy C-Means Clustering

FCM

- A method of clustering which allows one piece of data to belong to two or more clusters.

- Objective function to be minimized:

$$J_m = \sum_{i=1}^{N} \sum_{j=1}^{C} u_{ij}^m \left\| x_i - \mu_j \right\|^2, \qquad 1 \le m < \infty$$

Where

- u_{ij} is the degree of membership of x_j in the cluster j.
- x_i is d-dimensional observation
- μ_j is d-dimensional center of cluster j

Updation

- FCM is an iterative optimization approach.

- At each step, the membership u_{ij} and the cluster centers μ_j are updated as follows:

$$u_{ij} = \frac{1}{\sum_{k=1}^{c} \left(\frac{\|x_i - \mu_j\|}{\|x_i - \mu_k\|} \right)^{\frac{2}{m-1}}},$$

$$\mu_j = \frac{\sum_{i=1}^{N} u_{ij}^{m} . x_i}{\sum_{i=1}^{N} u_{ij}^{m}}$$

Termination Criterion

- Iteration stops, when

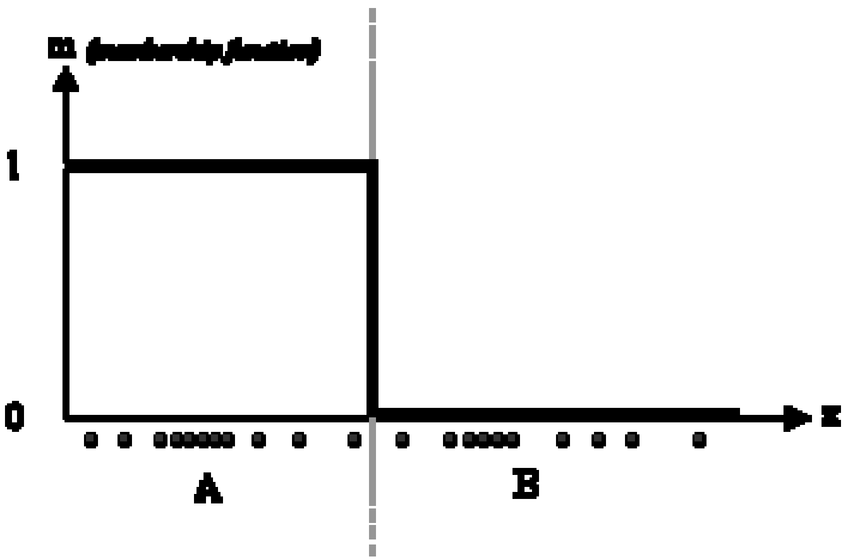
$$\max_{ij}\left\{\left|u_{ij}^{(k+1)} - u_{ij}^{(k)}\right|\right\} < \epsilon$$

Where k is the iteration number.

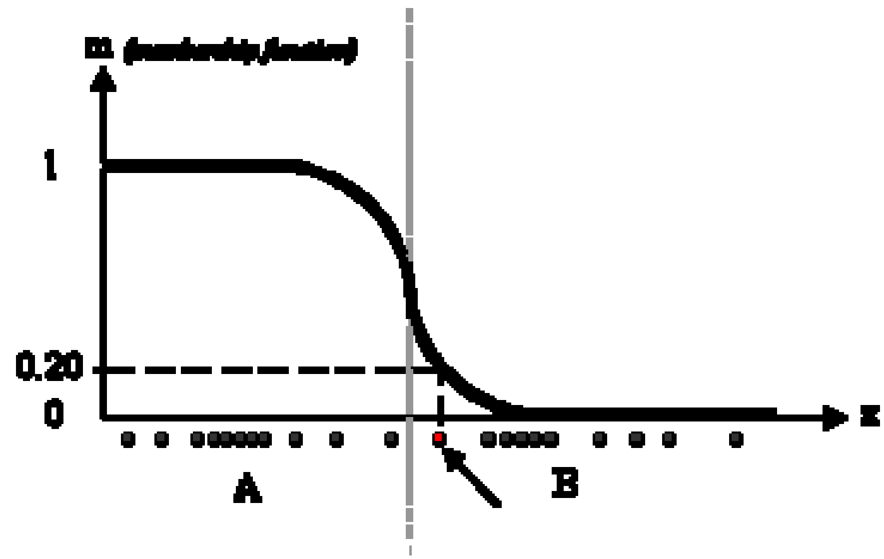
ϵ is between 0 and 1

K-means Vs FCM

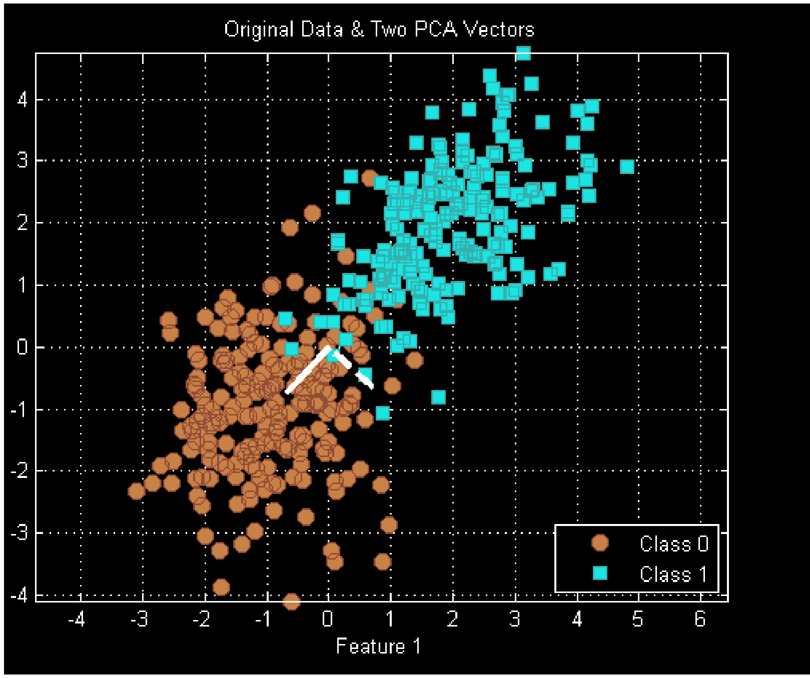
K-means

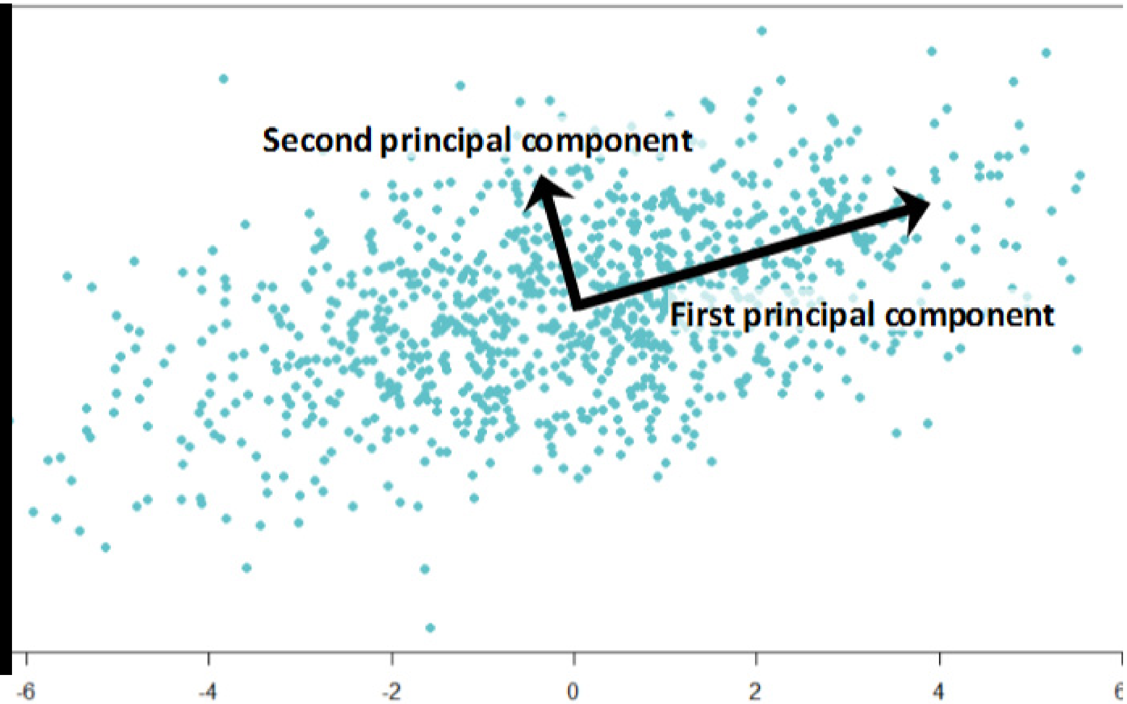


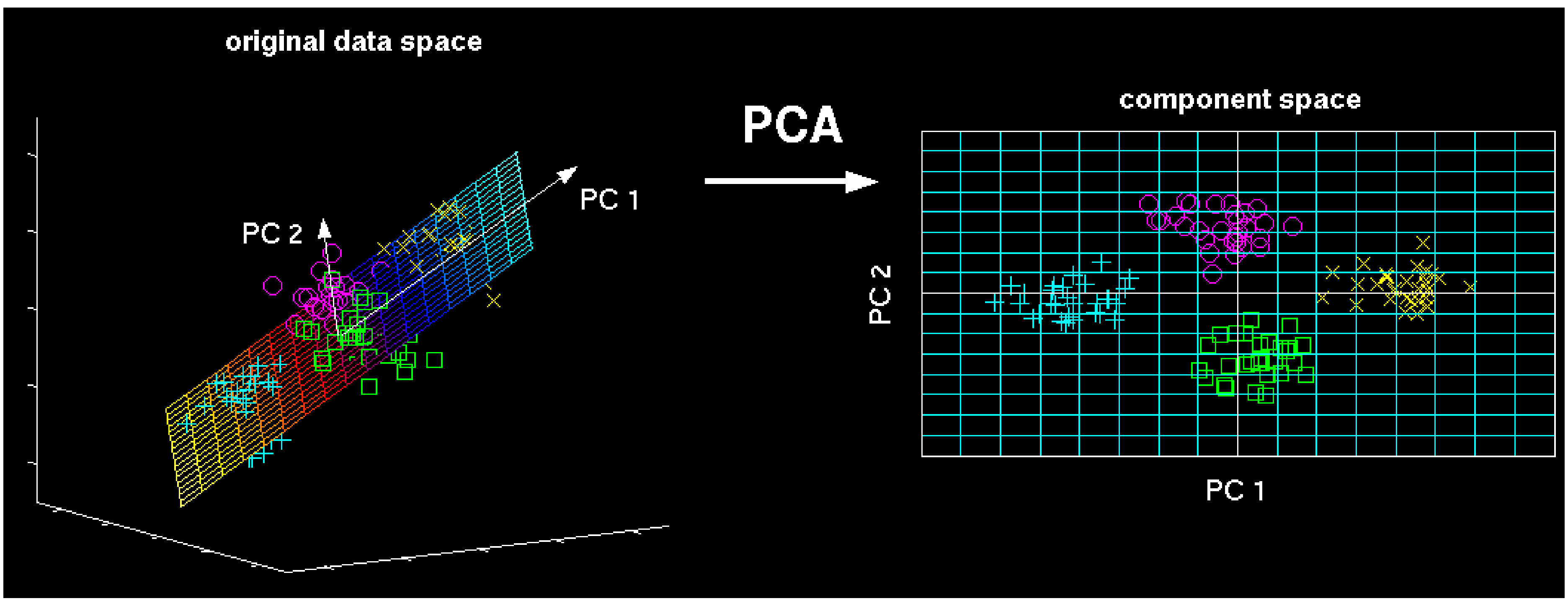
FCM



Read about K-medoids


Original Data & Two PCA Vectors
Feature 1
Class 0
Class 1


Second principal component
First principal component


original data space
PC 2
PC 1
PCA
component space
PC 2
PC 1

Hierarchical Clustering

Hierarchical Clustering

- Builds hierarchy of clusters

- Types:
  - Bottom Up - *Agglomerative*
    - *Starts by considering each observation as a cluster of it's own*
    - *Clusters are merged as we move up the hierarchy*
  - Top Down - *Divisive*
    - *Starts by considering all observations in one cluster*
    - *Clusters are divided as we move down the hierarchy*

Distance Functions

Certain mathematical properties are expected of any distance measure, or *metric*:

1. $d(x, y) \geq 0$ for all x, y.
2. $d(x, y) = 0$ iff $x = y$.
3. $d(x, y) = d(y, x)$ (symmetry)
4. $d(x, y) \leq d(x, z) + d(z, y)$ for all x, y, and z. (triangle inequality)

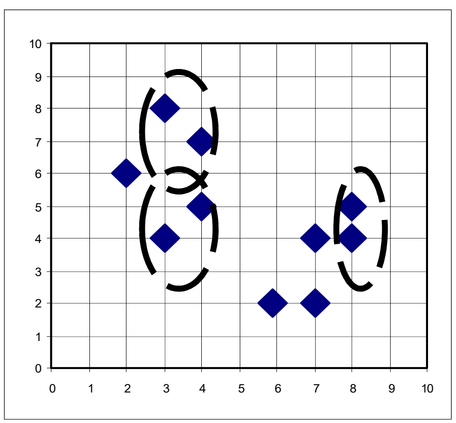
Euclidean distance $d(x, y) = \sqrt{\Sigma_{i=1}^{d} |x_i - y_i|^2}$ is probably the most commonly used metric. Note that it weights all features/dimensions "equally".

Some commonly used Metrics

- Euclidean distance
- Squared Euclidean distance
- Manhattan distance
- Maximum distance
- Mahalanobis distance

Agglomerative clustering

- Each node/object is a cluster initially
- Merge clusters that have the **least** dissimilarity
  - Ex: single-linkage, complete-linkage, etc.
- Go on in a non-descending fashion
- Eventually, all nodes belong to the same cluster



Linkage Criteria

- Determines the distance between sets of observations as a function of the pairwise distances between observations.

- Some commonly used criterias:
  - *Single Linkage:* Distance between two clusters is the **smallest** pairwise distance between two observations/nodes, each belonging to different clusters.

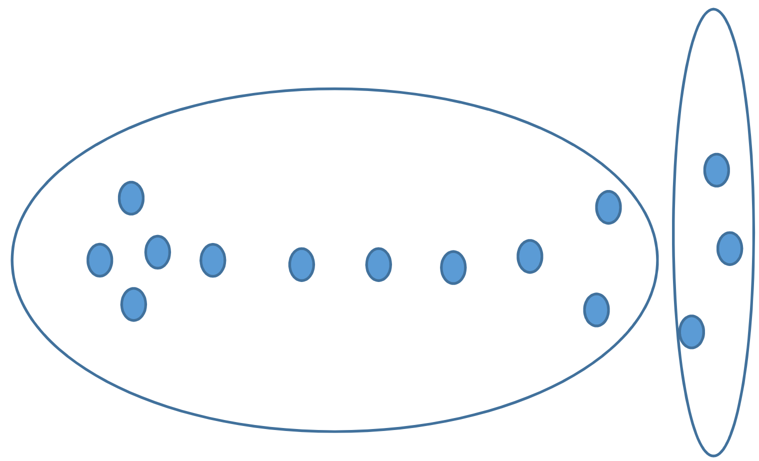
  - *Complete Linkage:* Distance between two clusters is the **largest** pairwise distance between two observations/nodes, each belonging to different clusters.

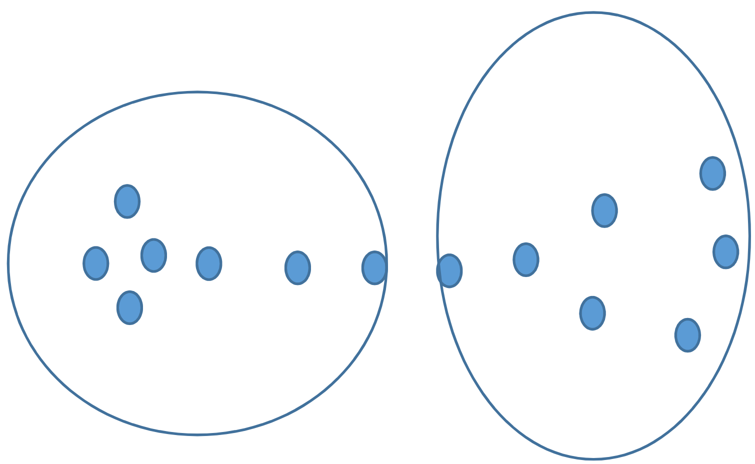
  - *Mean or average linkage clustering:* Distance between two clusters is the **average** of all the pairwise distances, each node/observation belonging to different clusters.

  - *Centroid linkage clustering:* Distance between two clusters is the **distance between their centroids**.

Single Linkage vs. Complete Linkage

Single linkage

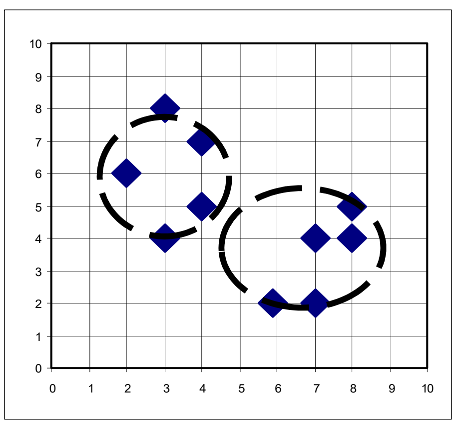




Complete linkage: Minimizes the diameter of the new cluster

Divisive Clustering

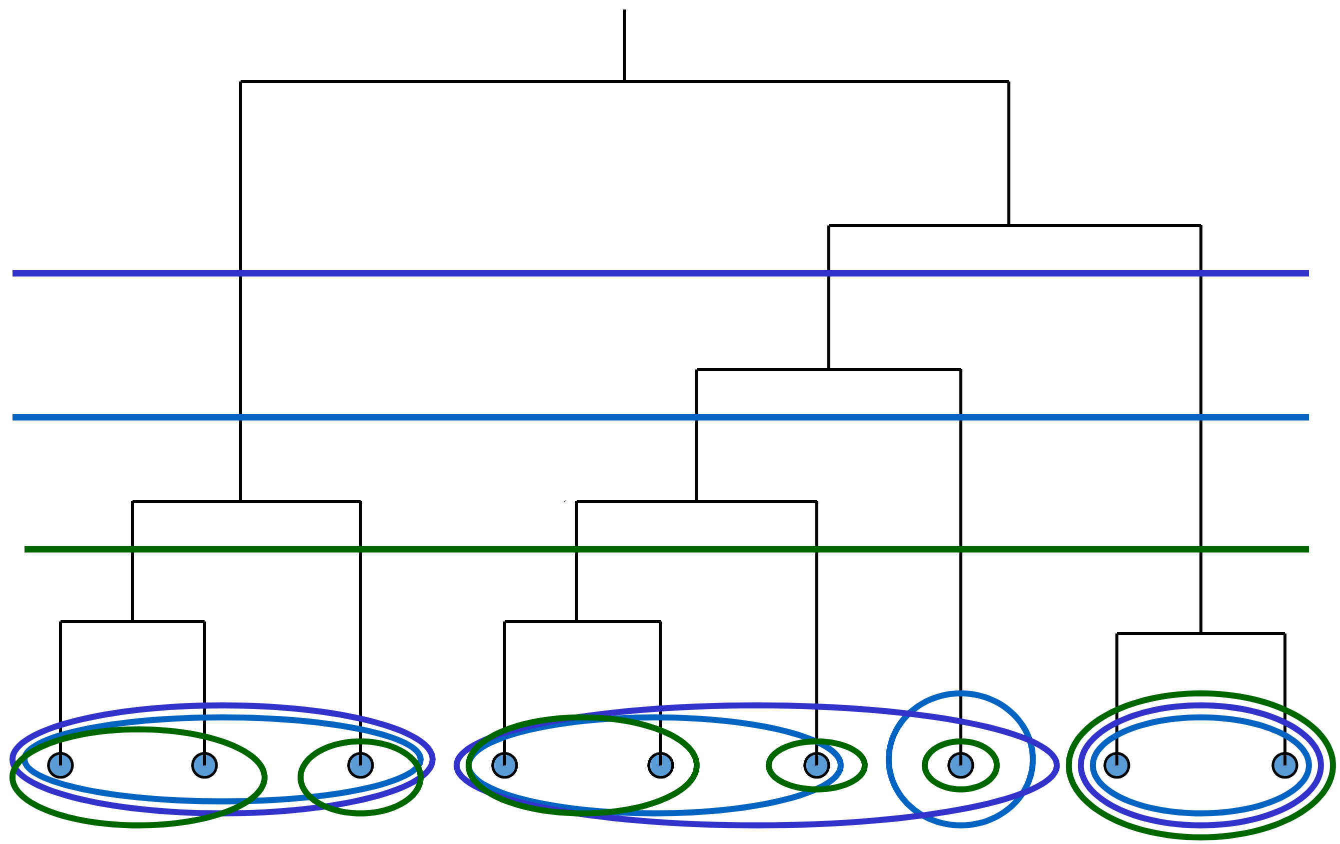
- Initially, all data is in the same cluster
- The largest cluster is split until every object is separate.



What are the true number of clusters?

- Decompose data objects into a several levels of nested partitioning (tree of clusters), called a dendrogram.

- A clustering of the data objects is obtained by cutting the dendrogram at the desired level, then each connected component forms a cluster.



DBSCAN : Density Based Spatial Clustering of Applications with Noise

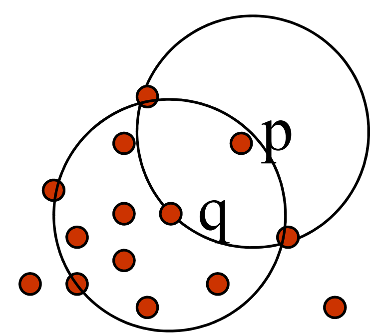
Density-Based Clustering Methods

- Clustering based on density (local cluster criterion), such as density-connected points
- Major features:
  - Discover clusters of arbitrary shape
  - Handle noise
  - Need density parameters as termination condition
- Several interesting studies:
  - DBSCAN: Ester, et al. (KDD'96)
  - OPTICS: Ankerst, et al (SIGMOD'99).
  - DENCLUE: Hinneburg & D. Keim (KDD'98)
  - CLIQUE: Agrawal, et al. (SIGMOD'98) (more grid-based)

Density-Based Clustering: Basic Concepts

- Two parameters:
  - *Eps*: Maximum radius of the neighborhood
  - *MinPts*: Minimum number of points in an *Eps*-neighborhood of that point
- $N_{Eps}(p)$: $\{q \text{ belongs to } D \mid dist(p,q) <= Eps\}$
- Directly density-reachable: A point *p* is directly density-reachable from a point *q* w.r.t. *Eps*, *MinPts* if
  - *p* belongs to $N_{Eps}(q)$
  - core point condition:

$$|N_{Eps}(q)| >= MinPts$$

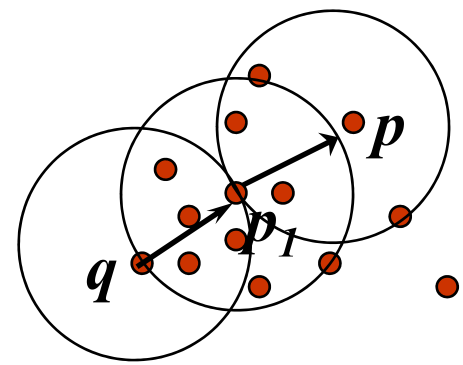


MinPts = 5

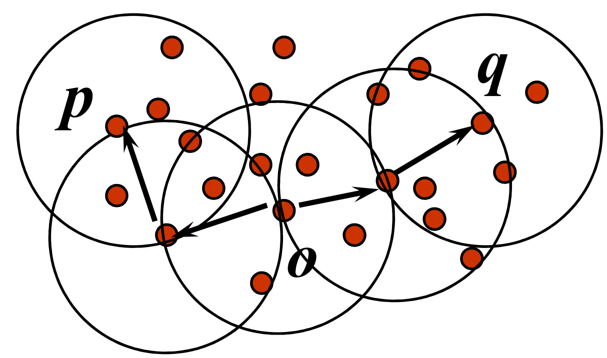
Eps = 1 cm

Density-reachable & Density-connected

- Density-reachable:
  - A point p is density-reachable from a point q if there is a chain of points $p_1, \ldots, p_n$, $p_1 = q$, $p_n = p$ such that p_{i+1} is directly density-reachable from p_i
  - This is not symmetric



- Density-connected
  - A point p is density-connected to a point q w.r.t. *Eps*, *MinPts* if there is a point o such that both, p and q are density-reachable from o w.r.t. *Eps* and *MinPts*

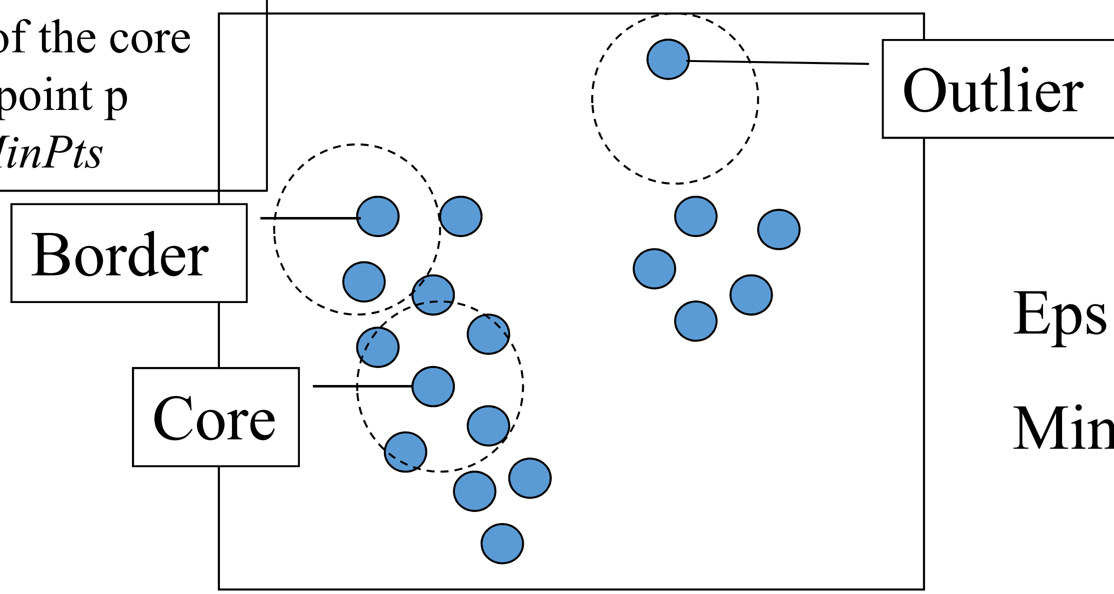


DBSCAN

- A set of points C is a cluster, if
  - For any two points $p, q \in C$, p and q are density-connected
  - There does not exist any pair of points, $p \in C$ and $s \notin C$ such that p and s are density-connected.

Border points are points that are reachable from any of the core points. For a border point p

$$|N_{Eps}(p)| < MinPts$$



Eps = 1cm

MinPts = 5

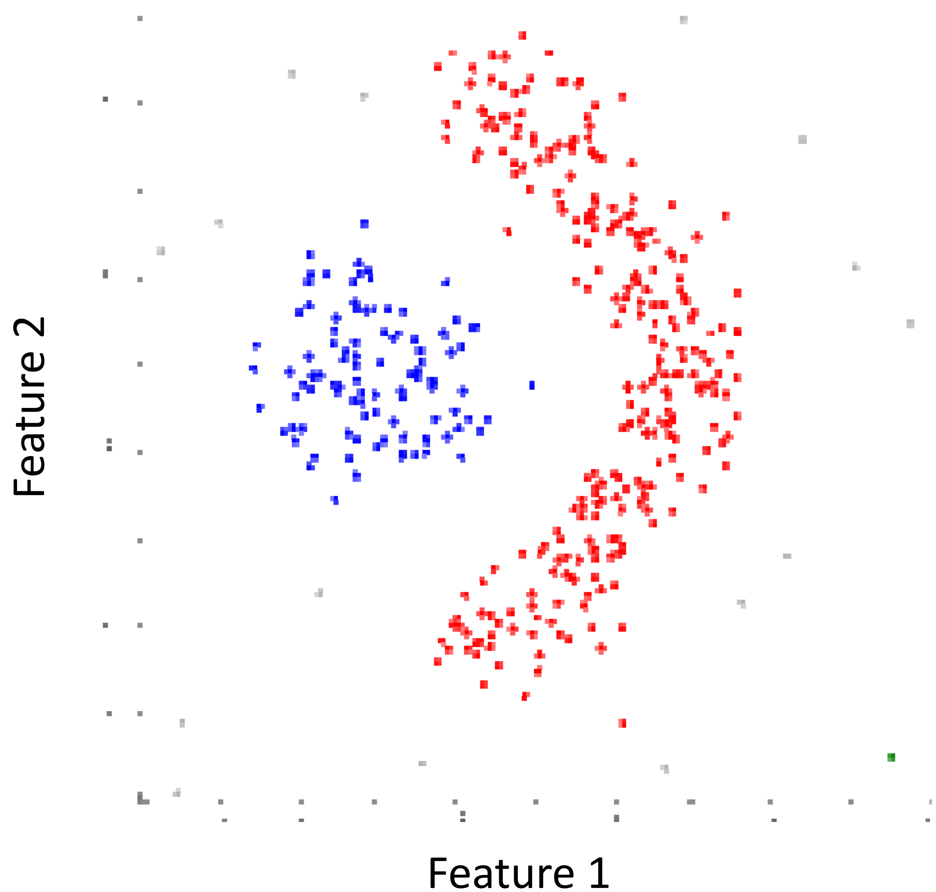
Algorithm

- **Select a point *p***
- **Retrieve all points directly density-reachable from *p* wrt. *Eps* and *MinPts*.**
- **If *p* is a not a core point, *p* is marked as noise**
- **Else a cluster is initiated.**
  - ***p* is marked as classified with a cluster ID**
  - ***seedSet* = all directly reachable points from *p.***
  - **For each point p_i in *seedSet* till it is empty**
    - **If p_i is a noise point, assign p_i to the current cluster ID**
    - **If p_i is unclassified, identify if it is a core point. If yes, then add all directly reachable point to seed set and add p_i to cluster ID**
    - **Delete p_i from *seedSet***

DBSCAN: Properties

- Can discover clusters of arbitrary shapes
- Complexity
  - Time
    - $O(n^2)$
    - $O(n\log^{d-1}n)$ with range tree. But requires more storage
      - d dimensions
- Weakness:
  - Parameter sensitive

DBSCAN - non-linearly separable clusters



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