CLUSTERING
Methods

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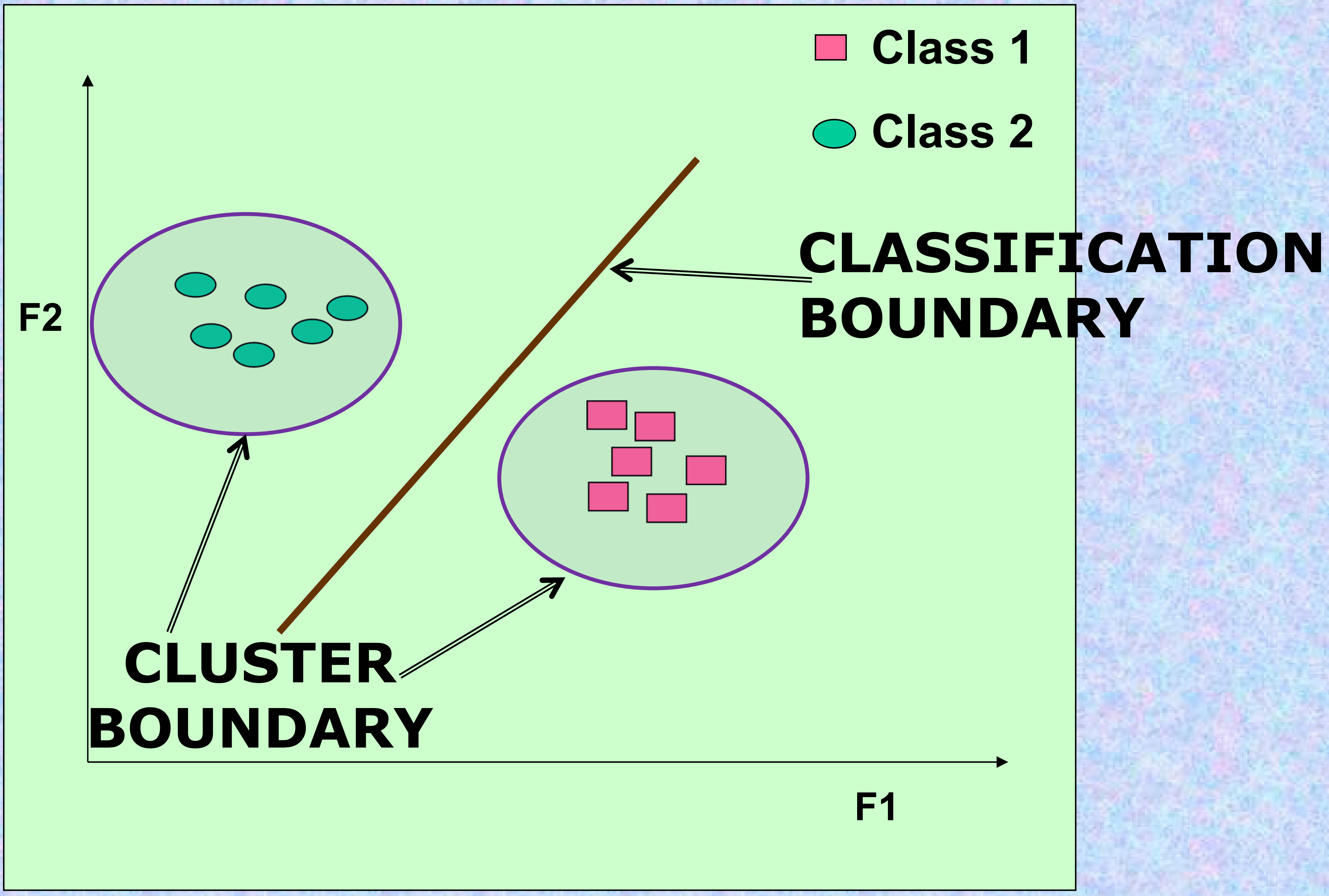
What is Cluster Analysis?

- 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

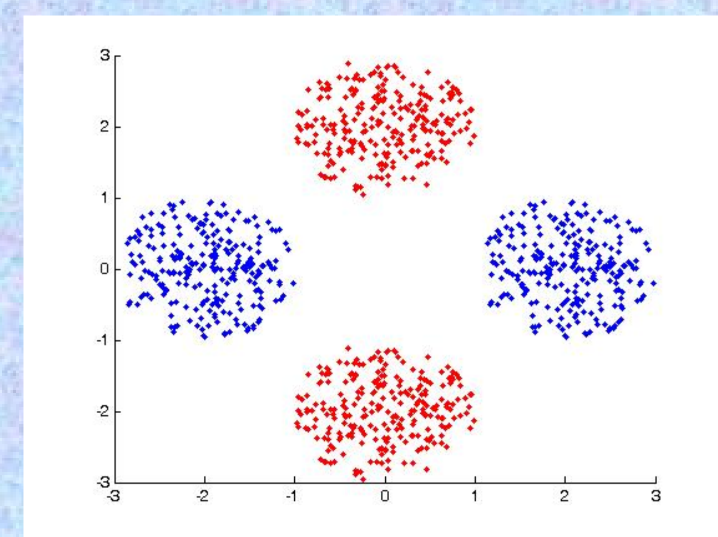
Clustering: Application Examples

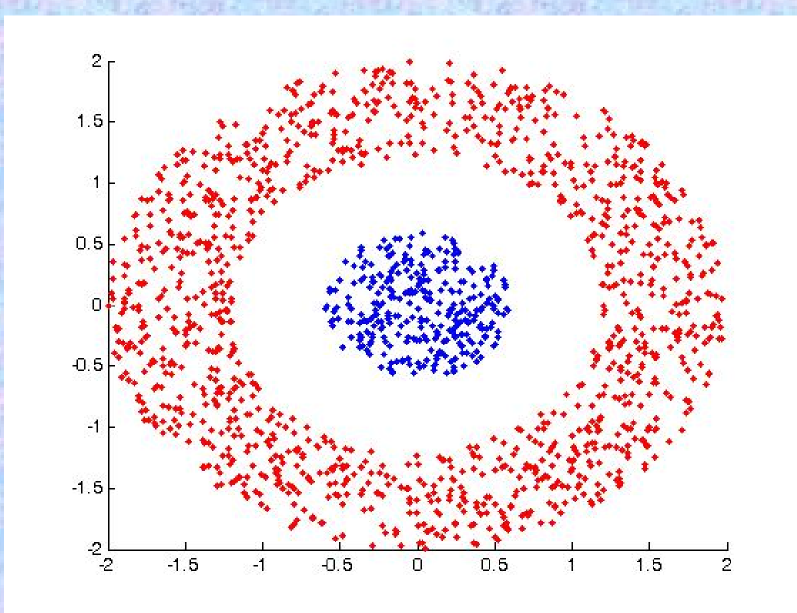
- **Biology**: taxonomy of living things: kingdom, phylum, class, order, family, genus and species
- **Information retrieval**: document clustering
- **Land use**: Identification of areas of similar land use in an earth observation database
- **Marketing**: Help marketers discover distinct groups in 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

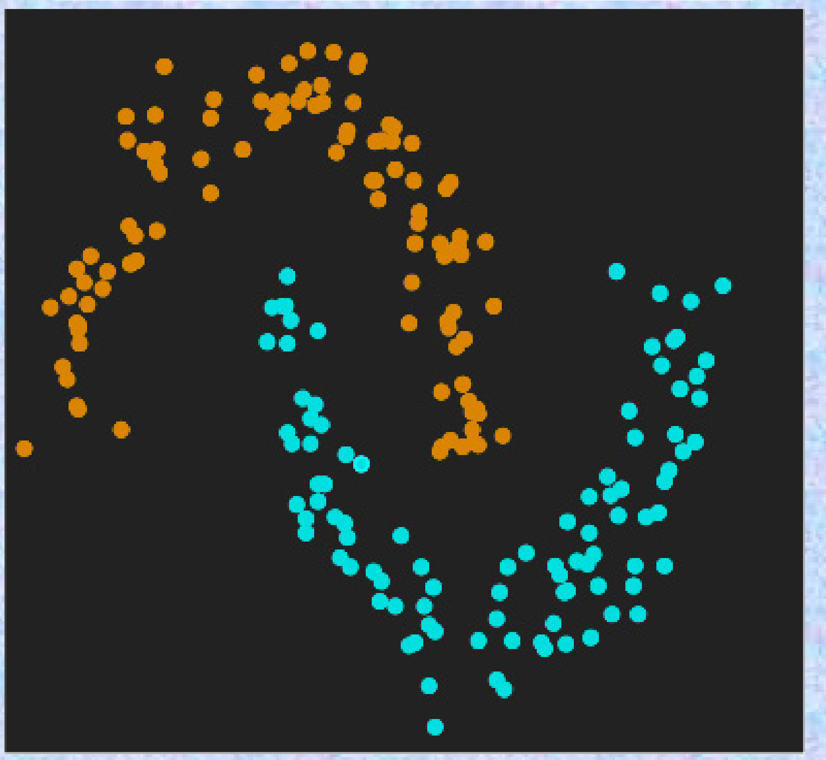


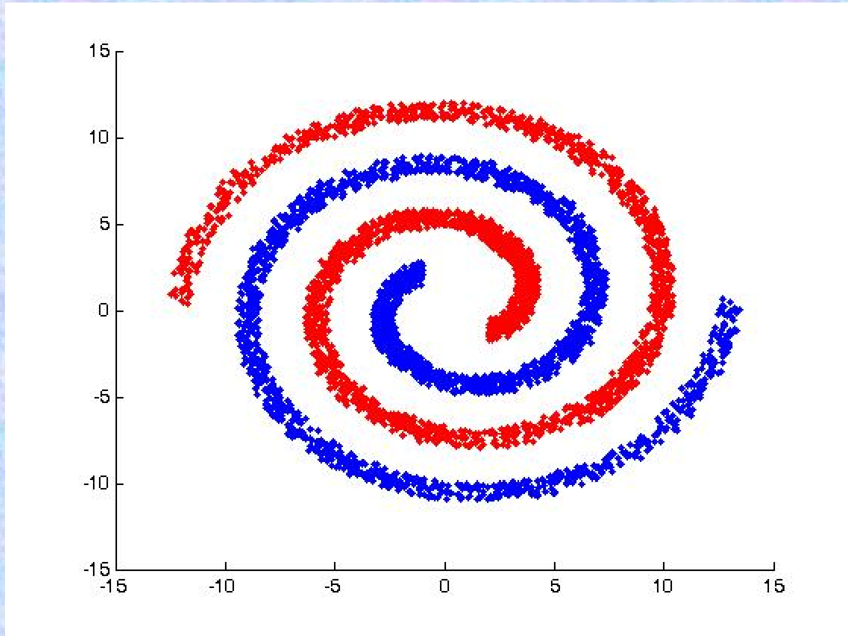
Sample points in a two-dimensional feature space

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)

- <u>Model-based</u>:
  - 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
- <u>Frequent pattern-based:</u>
  - Based on the analysis of frequent patterns
  - Typical methods: p-Cluster
- <u>User-guided or constraint-based</u>:
  - Clustering by considering user-specified or application-specific constraints
  - Typical methods: COD (obstacles), constrained clustering
- <u>Link-based clustering</u>:
  - 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

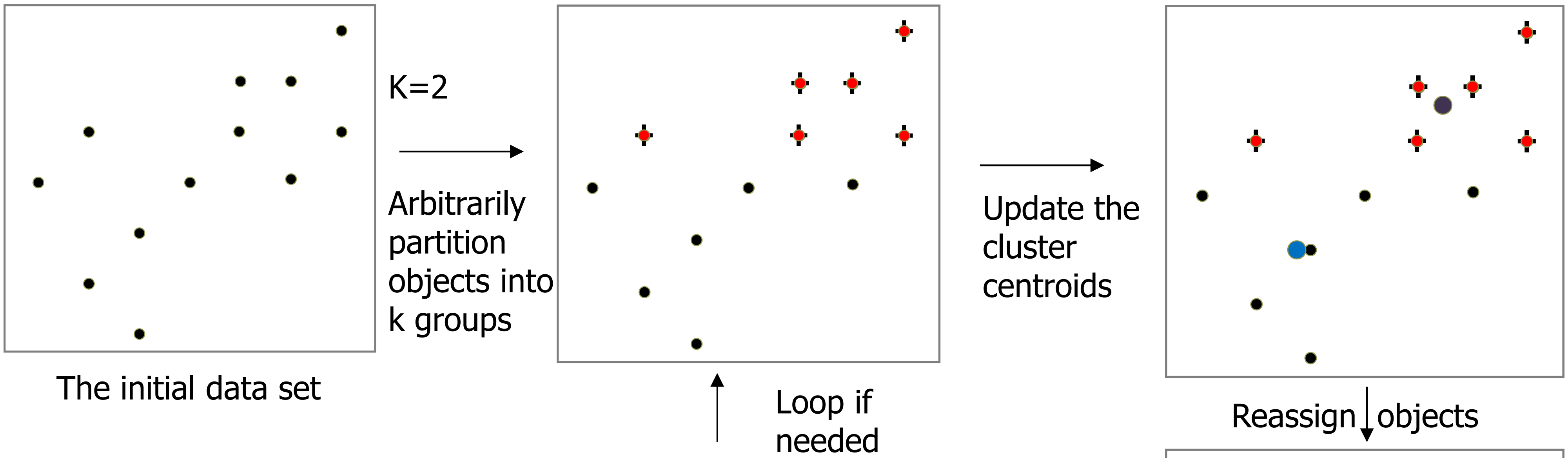
Alternative view of Algorithms for CLUSTERING

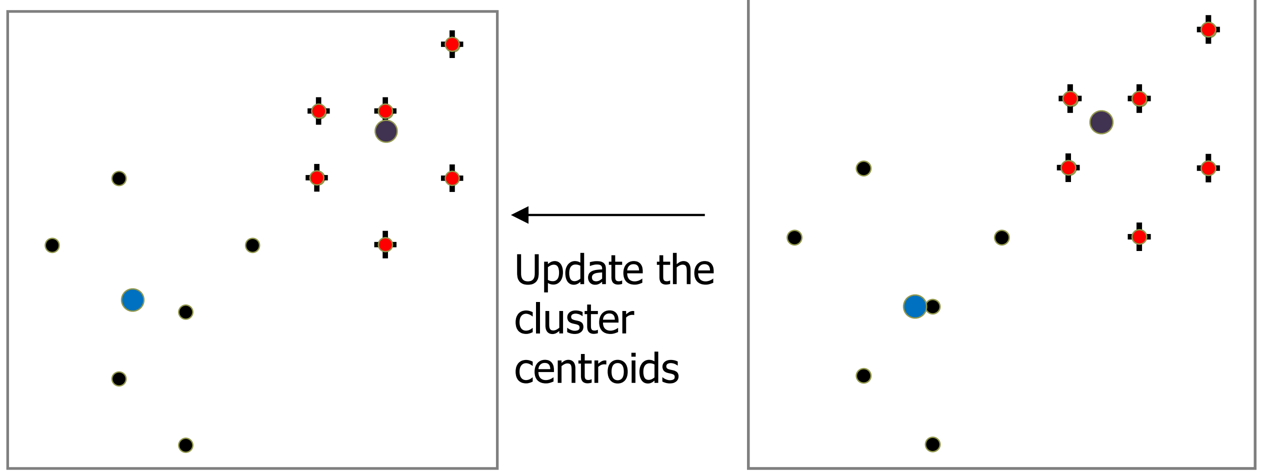
- Unupervised Learning/Classification:
  - K-means; K-medoid

- 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)

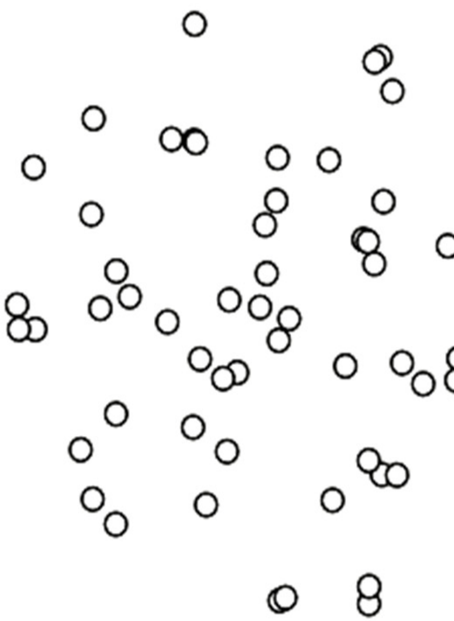
- **Density Estimation :**
  (ii) Non-Parametric
  - **Histogram**
  - **Neighborhood**
  - **Kernel Methods**
  - **Graph Theoretic**
  - **Iterative Valley Seeking**

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:

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

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:

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

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

Let C = 3; d = 2;
Class Means on vertices of an Equilateral Triangle.

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

μ_1

x_i

μ_2 μ_3

$u_{ij} = 1/3$

$m > 1$

$l = 2/(m-1)$

u_{i1}

$u_{i2/3} =$

Let C = 3; d = 2;
Class Means on vertices of an Equilateral Triangle.

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

μ_1

$\otimes X_i$

μ_2 μ_3

$$u_{ij} = 1/3$$

$m > 1$

$\ell = 2/(m-1)$

μ_1

$\otimes X_i$

μ_2 μ_3

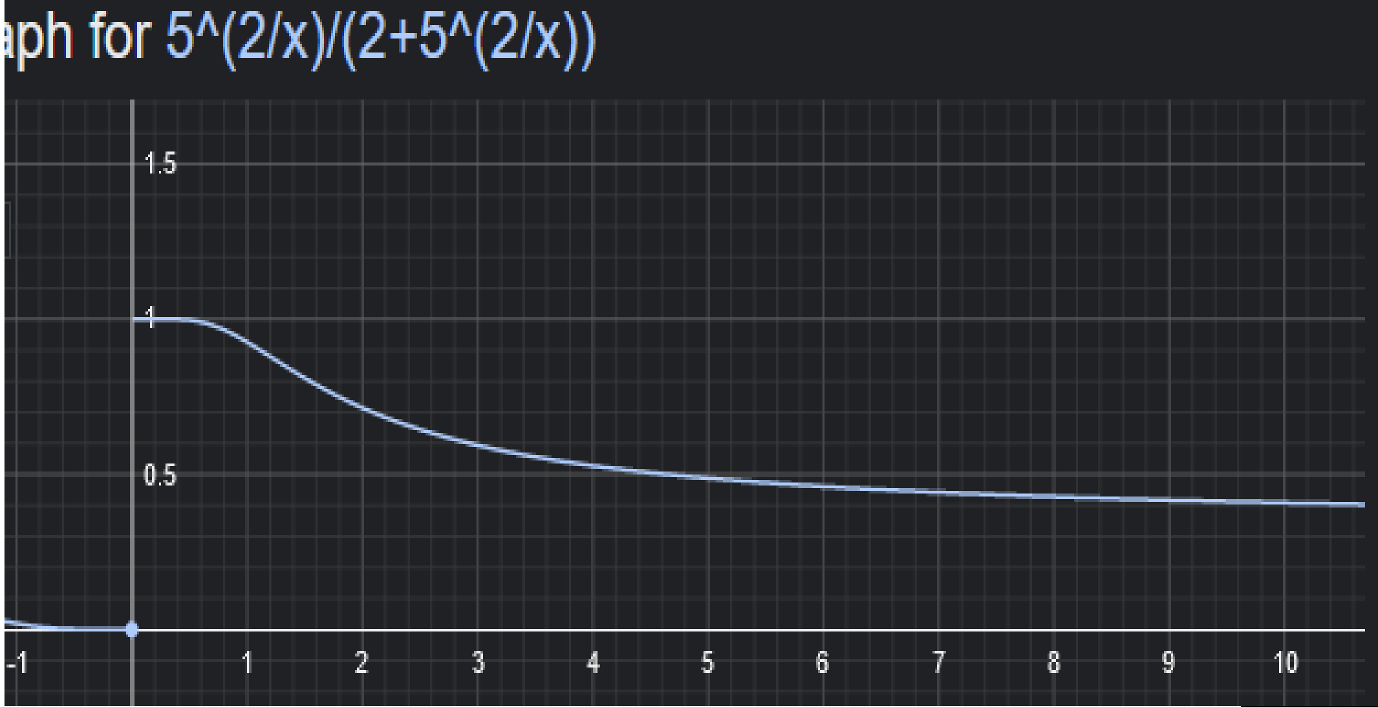
$$\alpha = \frac{|X_i - \mu_k|}{|X_i - \mu_j|} \quad k \neq j$$

$$u_{i1} = \frac{1}{1 + \left(\frac{1}{\alpha}\right)^{\ell} + \left(\frac{1}{\alpha}\right)^{\ell}} = \frac{\alpha^{\ell}}{\alpha^{\ell} + 2} \simeq 1 \qquad \alpha \gg 1$$

$$u_{i2/3} = \frac{1}{\left(\frac{1}{\alpha}\right)^{\ell} + 1 + 1} \qquad \alpha \ll 1 \qquad \simeq \alpha^{\ell}$$

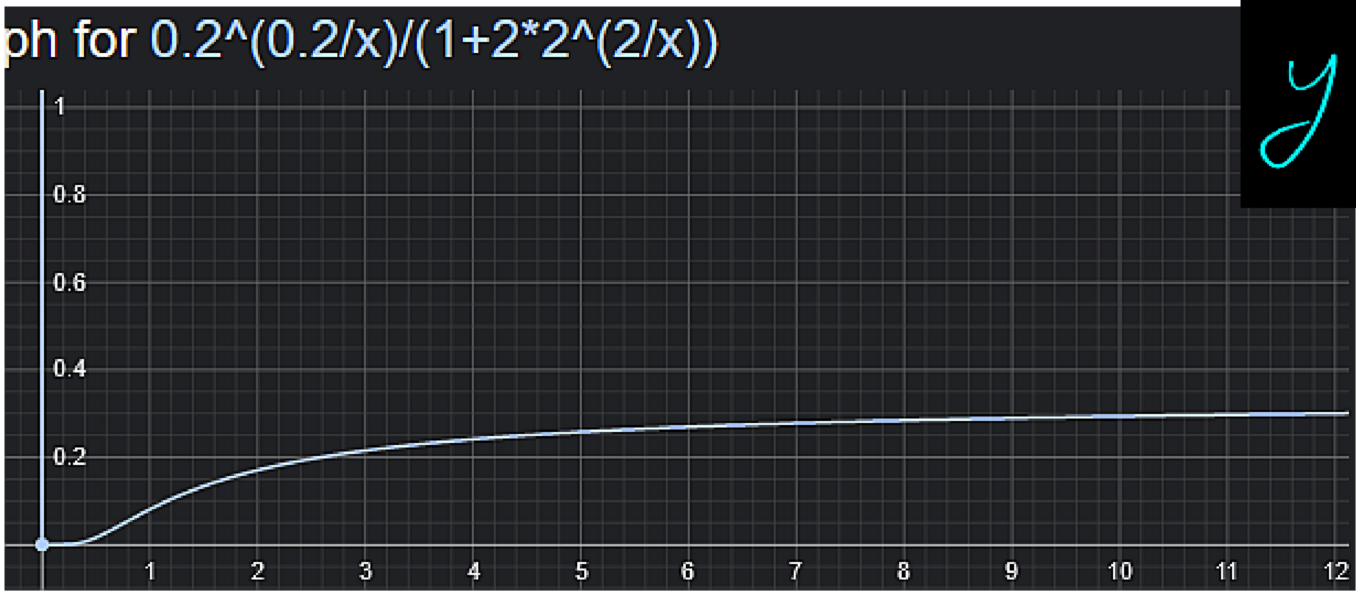
Go ahead; Plot them

U vs x = (m-1)



$$y = \frac{5^{2/x}}{2+5^{2/x}}$$

$$y = \frac{0.2^{2/x}}{1+2\left(2^{2/x}\right)}$$



Termination Criterion

- Iteration stops, when

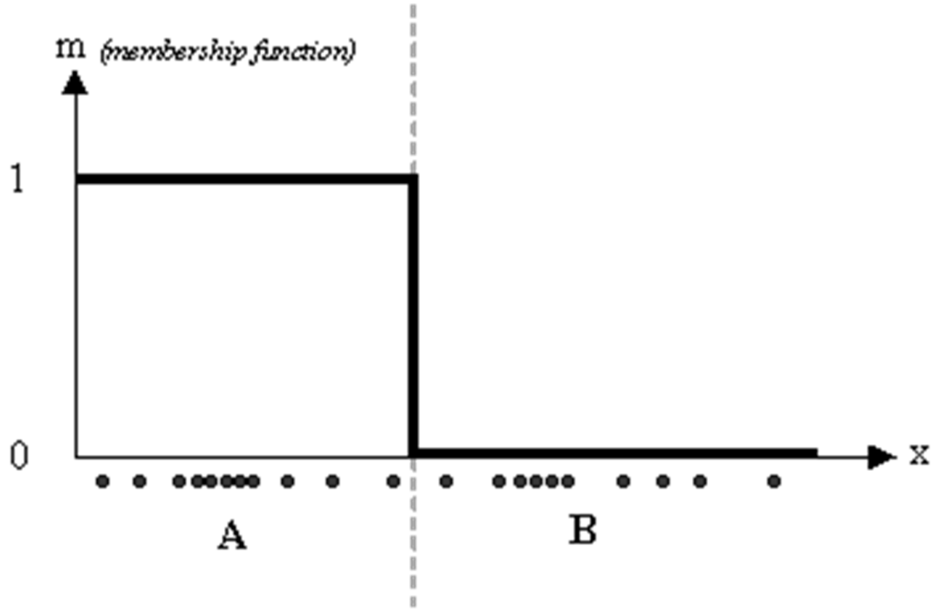
$$\max_{ij}\left\{\left|u_{ij}^{(k+1)} - u_{ij}^{(k)}\right|\right\} < \epsilon$$

Where k is the iteration number.

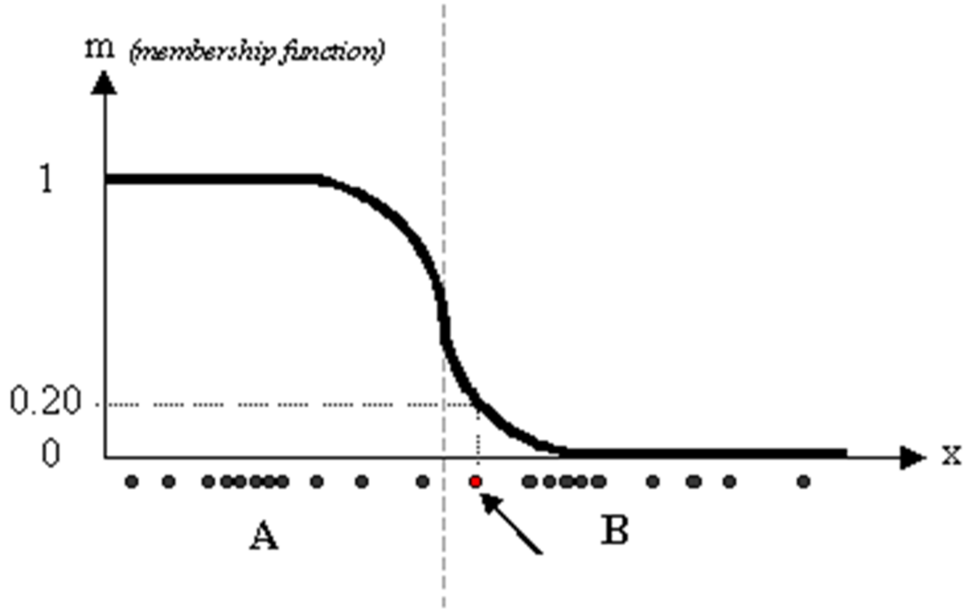
ϵ is between 0 and 1

K-means Vs FCM

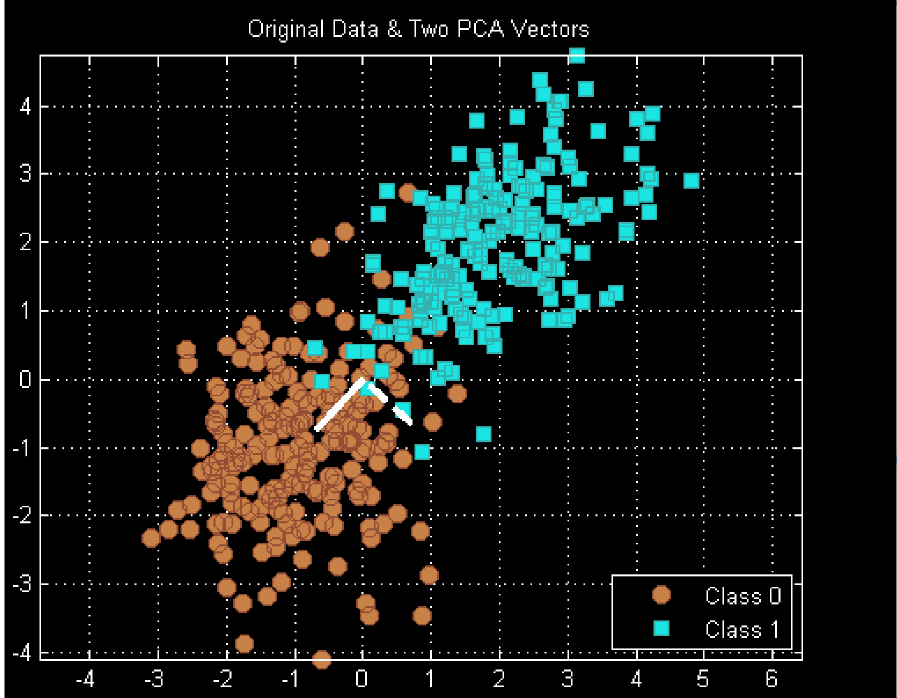
K-means

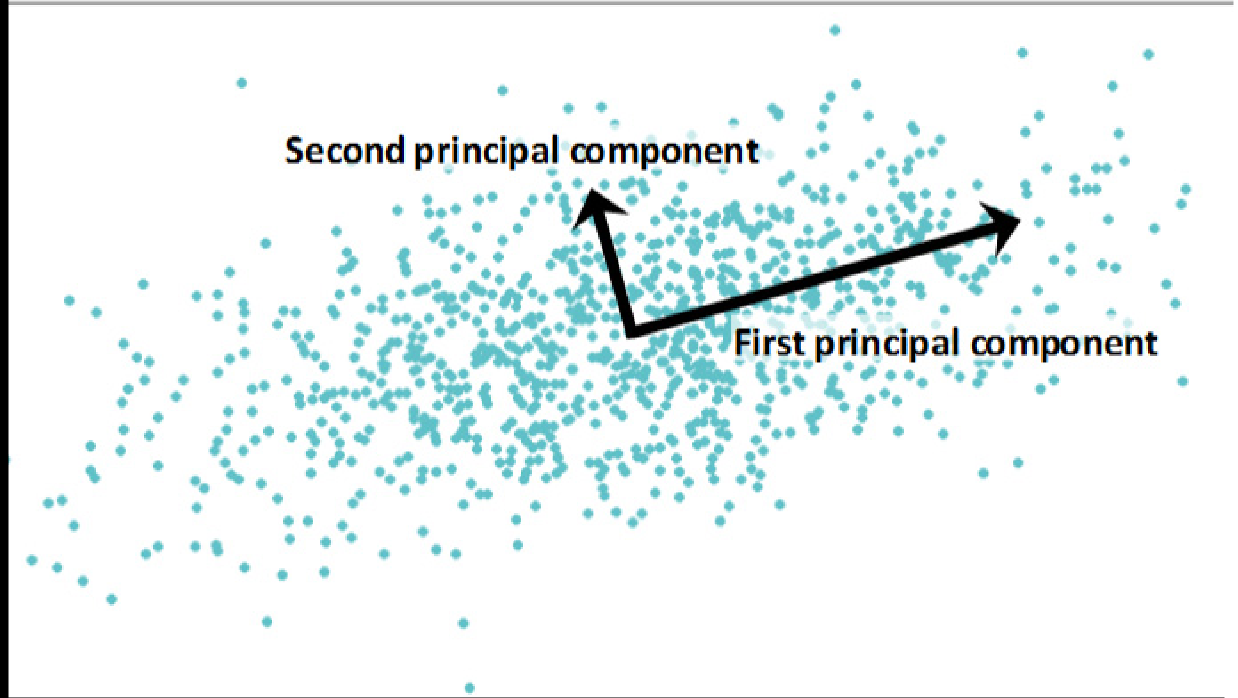


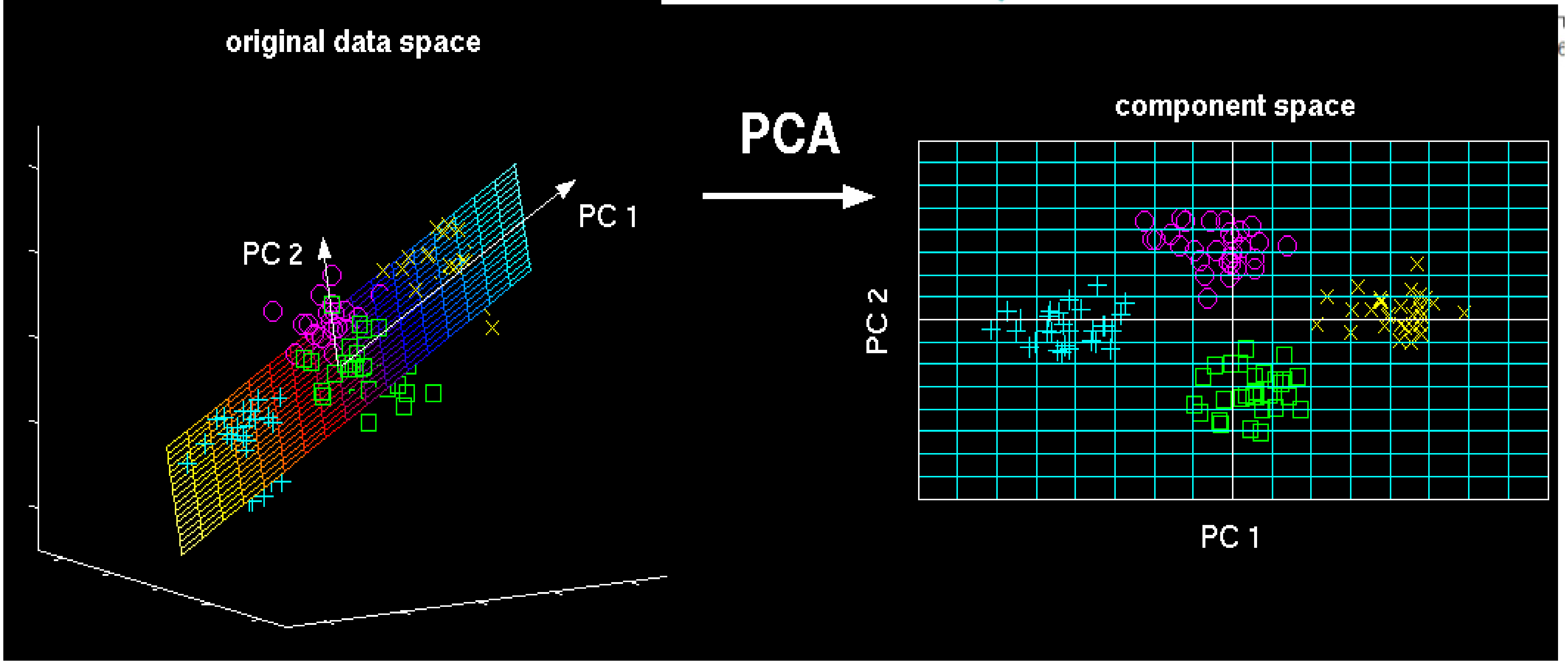
FCM

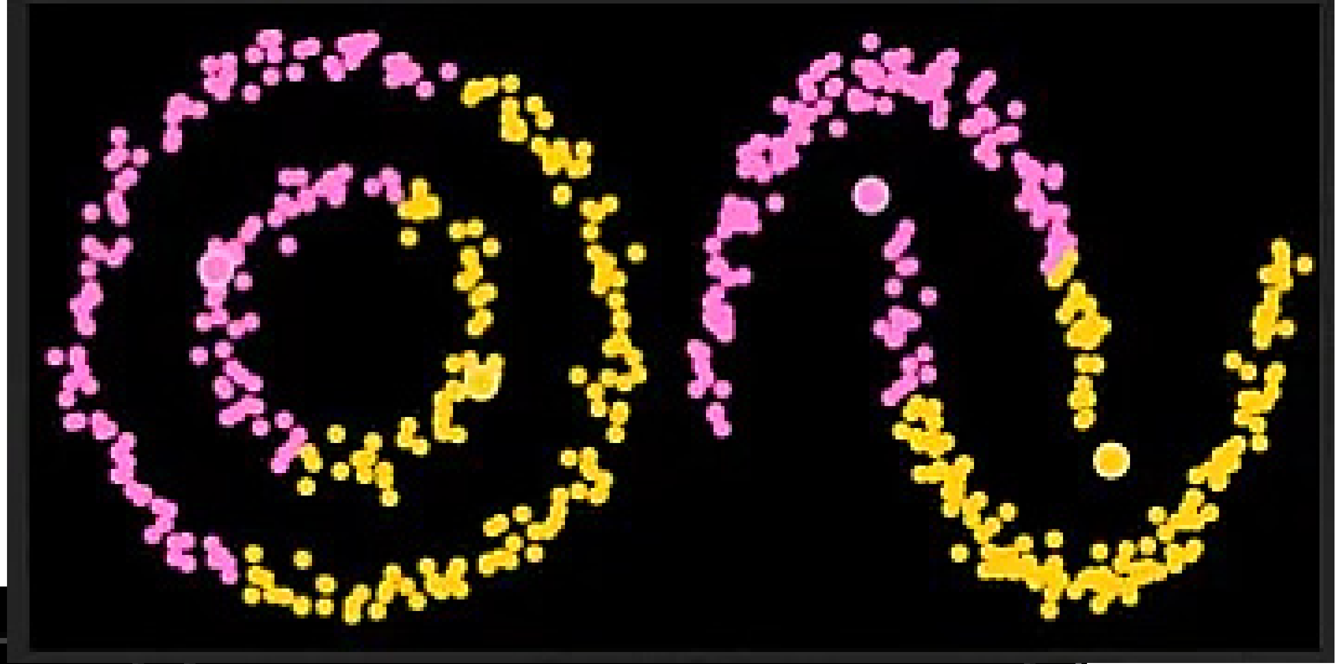


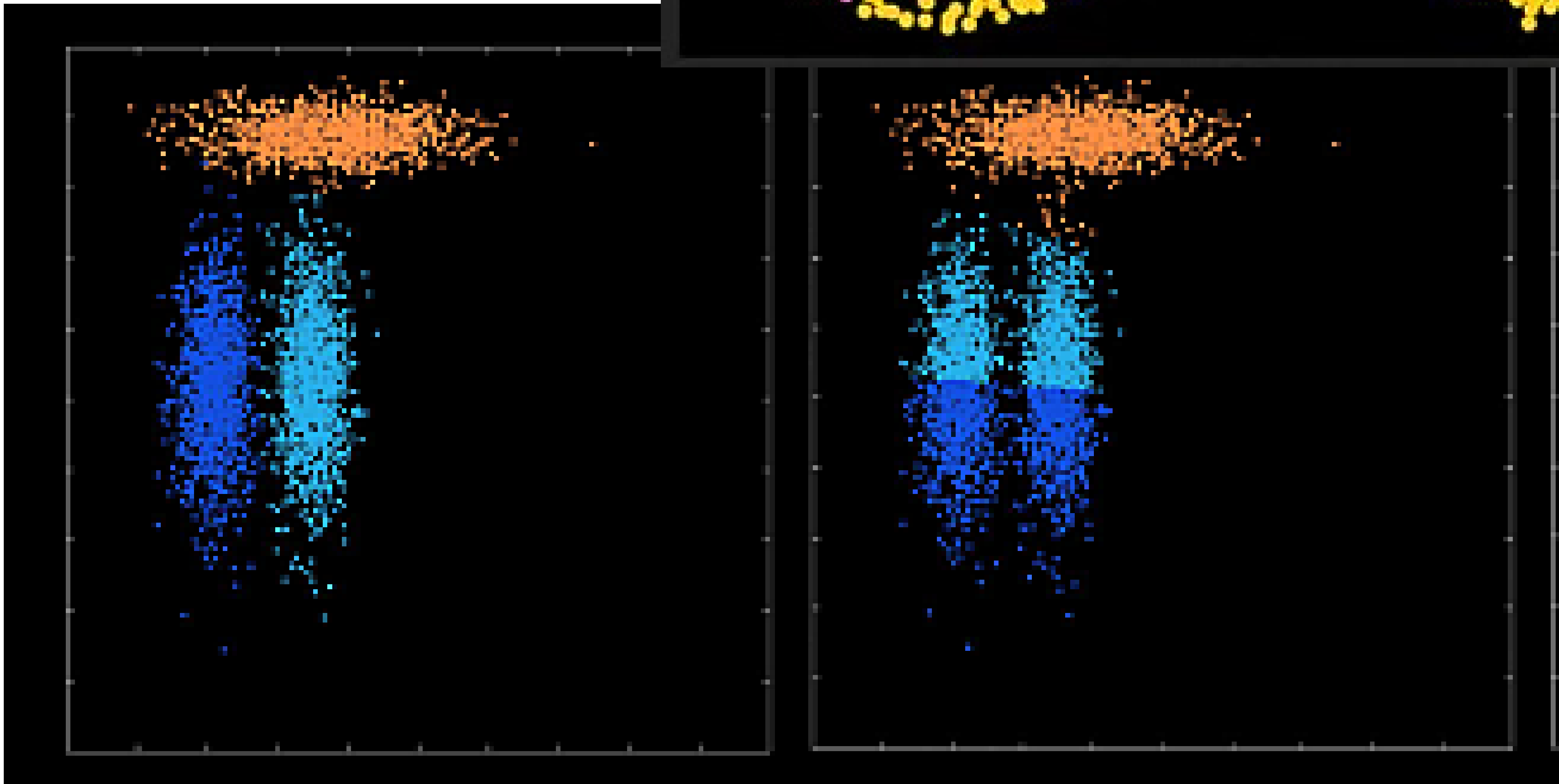
Read about K-medoids


Original Data & Two PCA Vectors
Class 0
Class 1


Second principal component
First principal component


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





(a) Generated synthetic data (b) K-means

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)

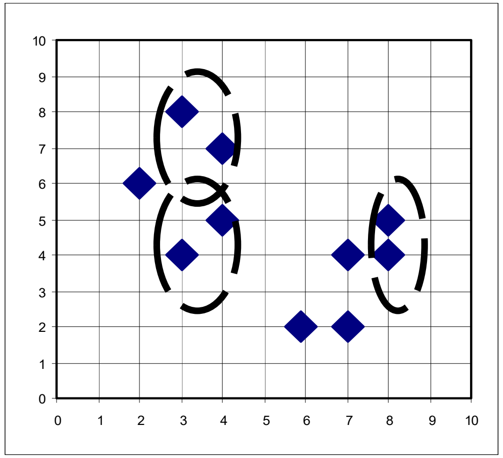
Euclidean distance $d(x, y) = \sqrt{\Sigma_{i=1}^{d} |x_i - y_i|^2}$ is probably the most commonly used metric. Note that it weights all features/dimensions "equally".

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

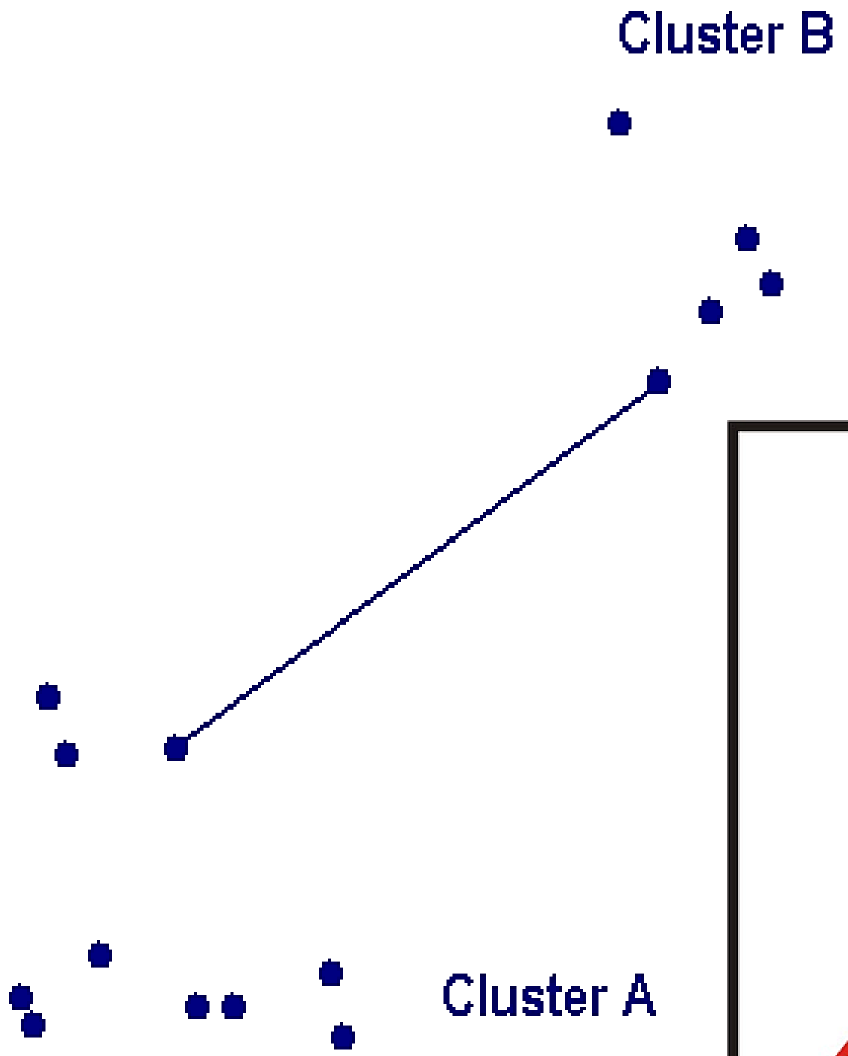
- Determines the distance between sets of observations as a function of the pairwise distances between observations.

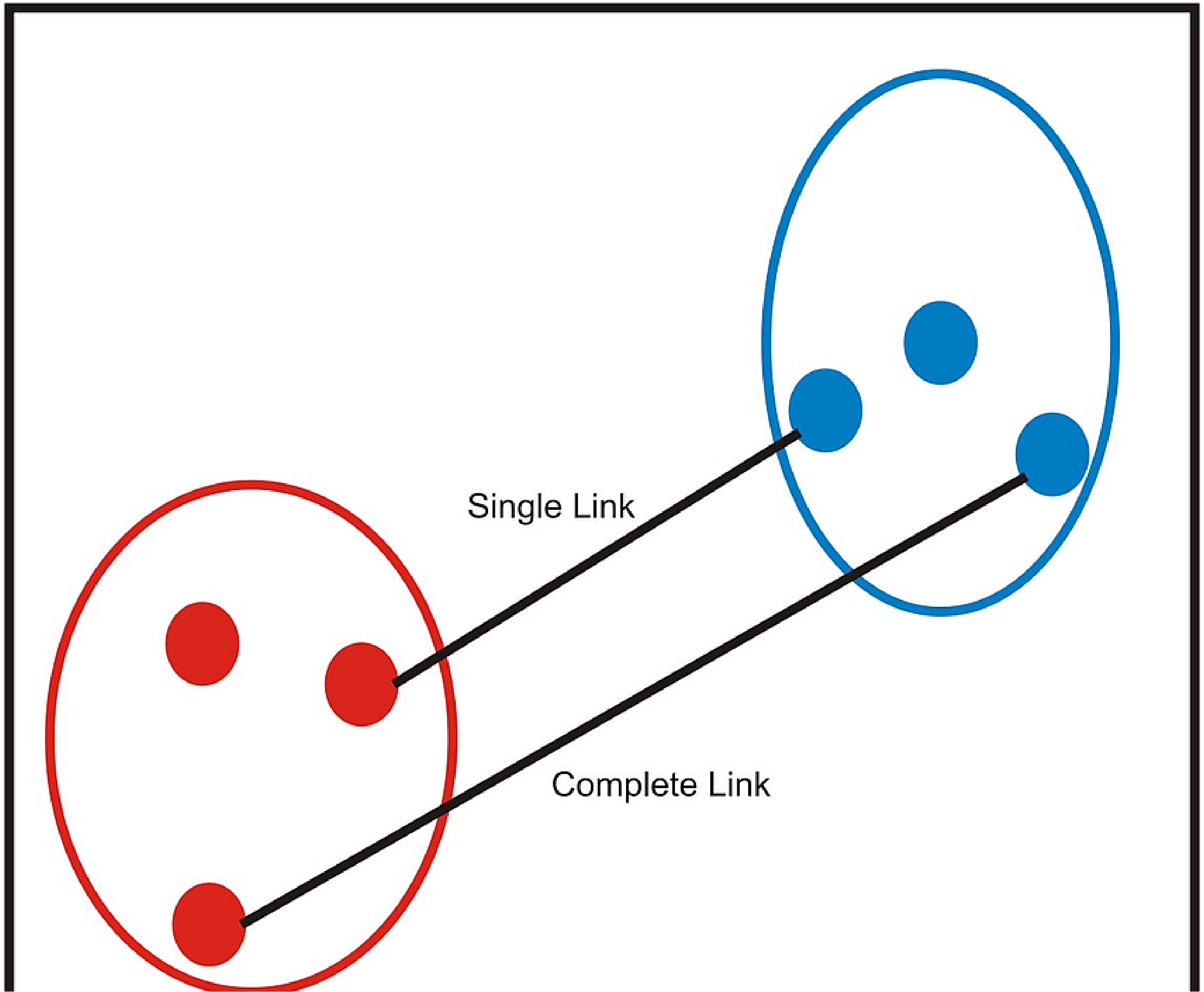
- Some commonly used criterias:
  - *Single Linkage:* Distance between two clusters is the **smallest** pairwise distance between two observations/nodes, each belonging to different clusters.

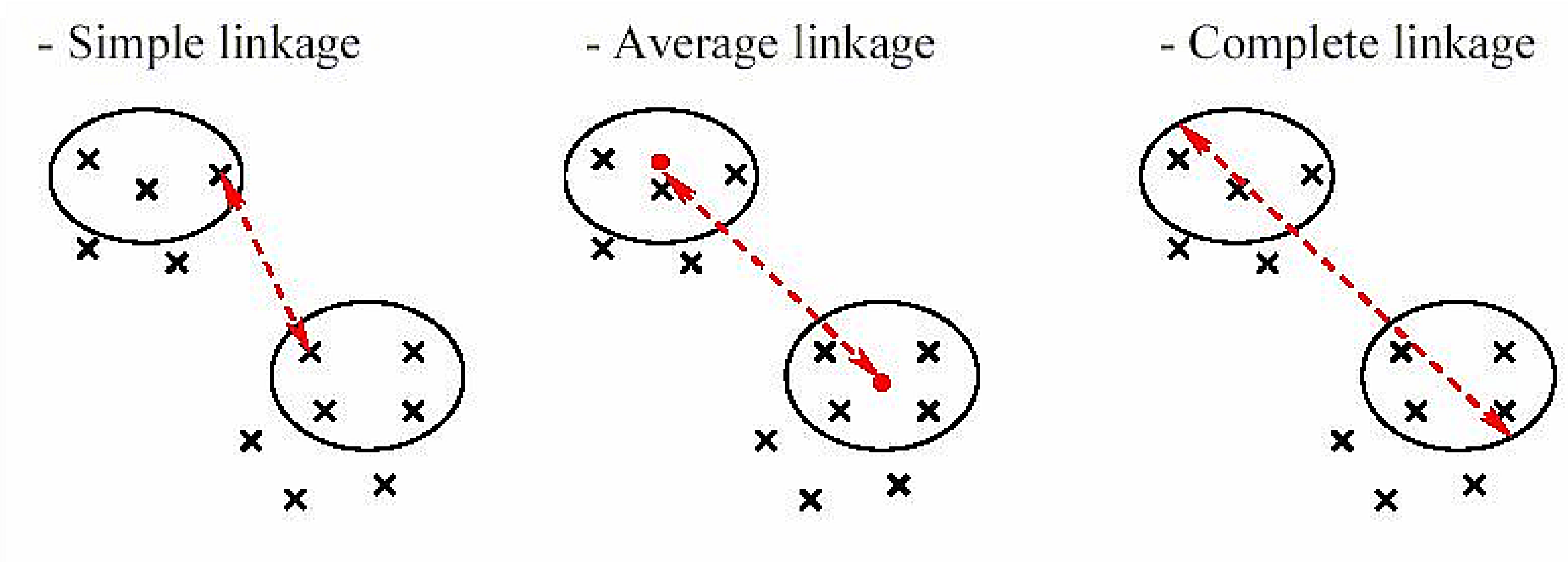
  - *Complete Linkage:* Distance between two clusters is the **largest** pairwise distance between two observations/nodes, each belonging to different clusters.

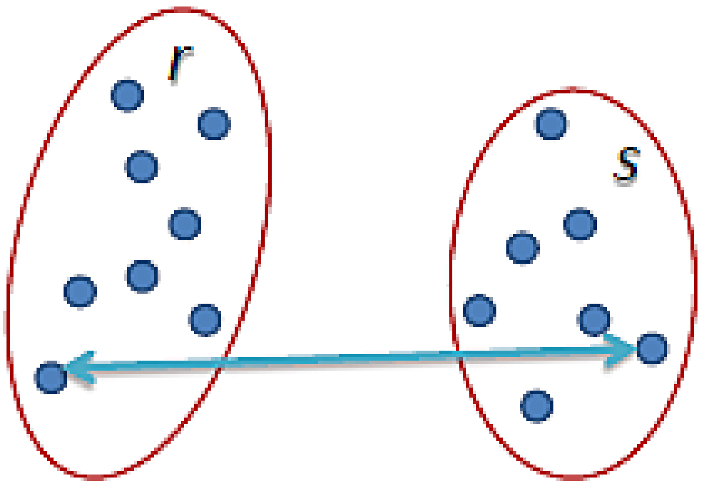
  - *Mean or average linkage clustering:* Distance between two clusters is the **average** of all the pairwise distances, each node/observation belonging to different clusters.

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

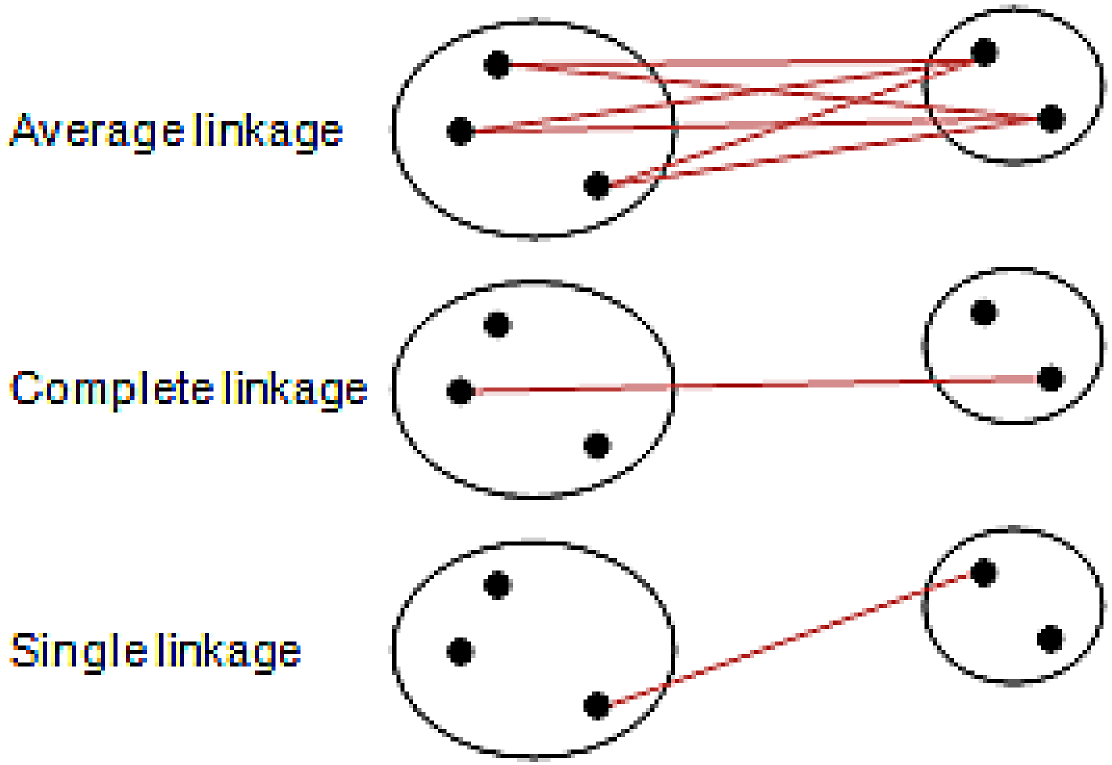

Cluster B
Cluster A


Single Link
Complete Link



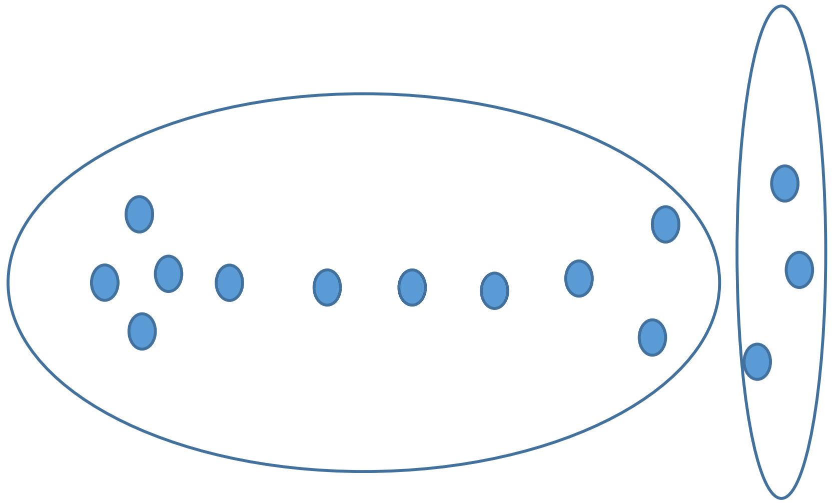


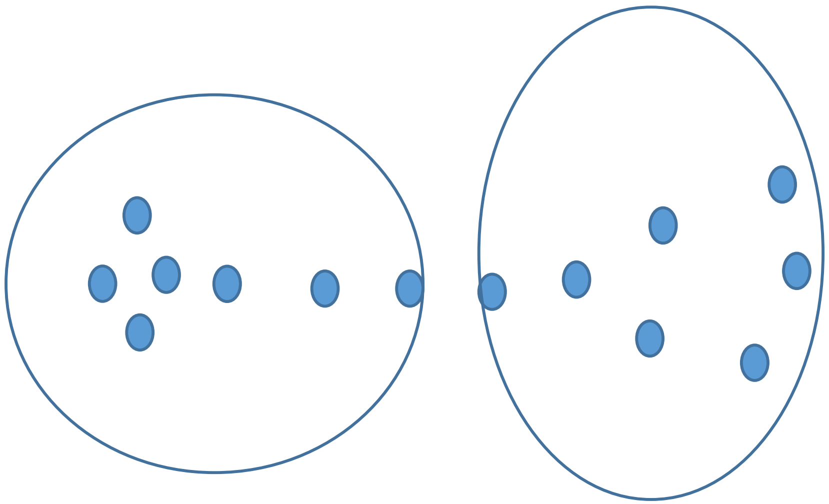
$$L(r,s) = \max(D(x_{ri}, x_{sj}))$$



Single Linkage vs. Complete Linkage

Single linkage

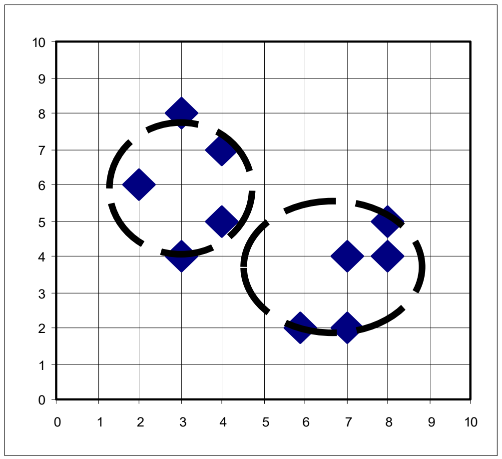




Complete linkage: Minimizes the diameter of the new cluster

Divisive Clustering

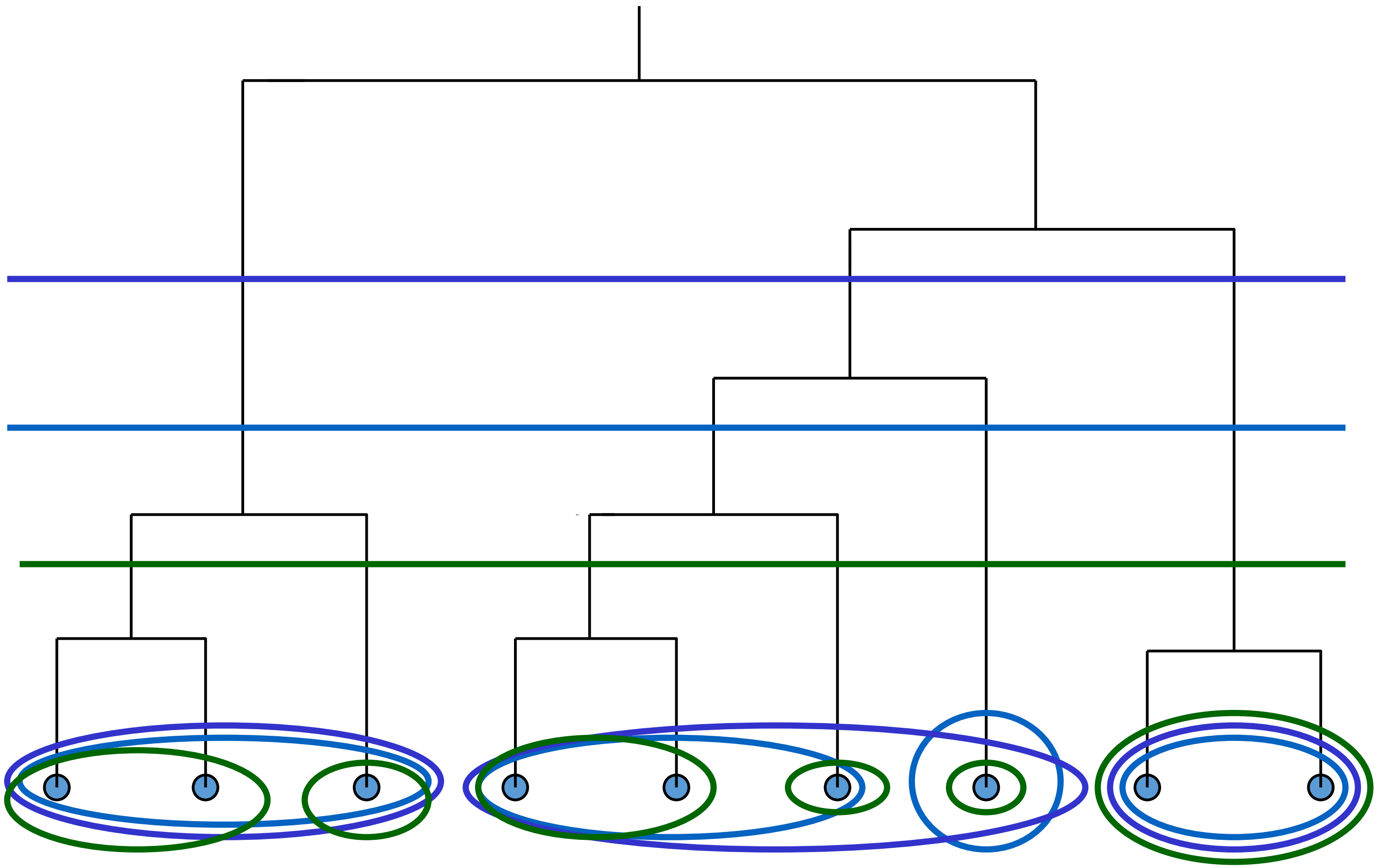
- Initially, all data is in the same cluster
- The largest cluster is split until every object is separate.

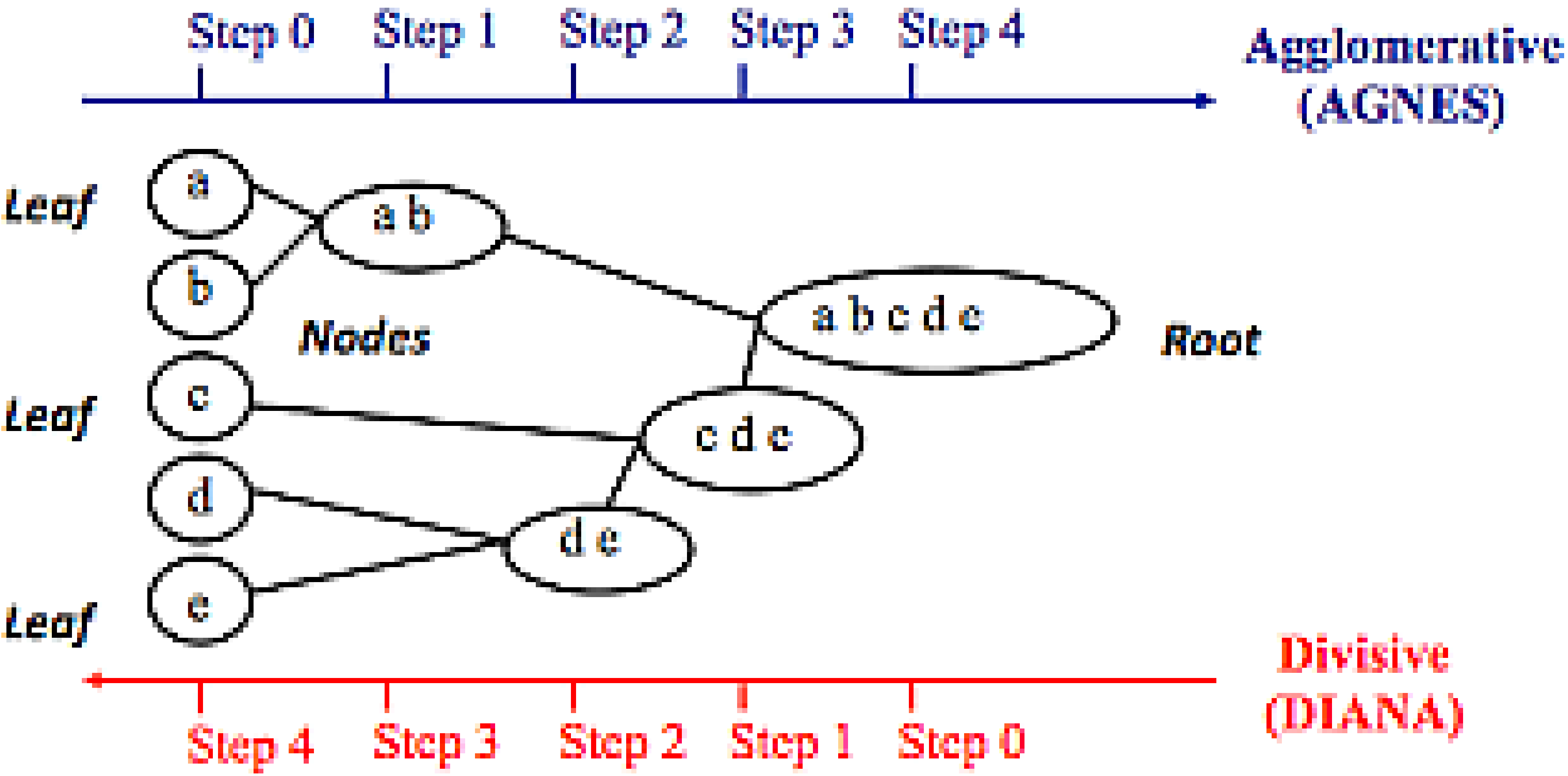


What are the true number of clusters?

- 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.




Step 0
Step 1
Step 2
Step 3
Step 4
Agglomerative
(AGNES)
Leaf
Leaf
Leaf
Nodes
Root
a
b
c
d
e
a b
a b c d e
c d e
d e
Divisive
(DIANA)
Step 4
Step 3
Step 2
Step 1
Step 0

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

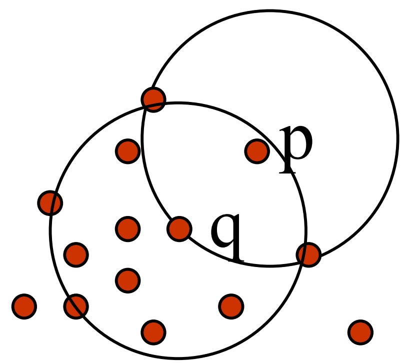
- Major features:
  - Discover clusters of arbitrary shape
  - Handle noise
  - Need density parameters as termination condition

- 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:

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

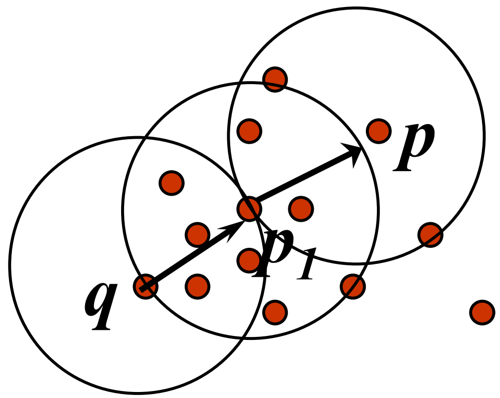


MinPts = 5

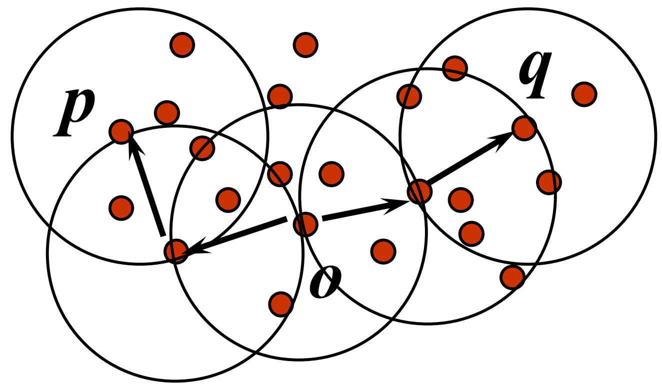
Eps = 1 cm

Density-reachable & Density-connected

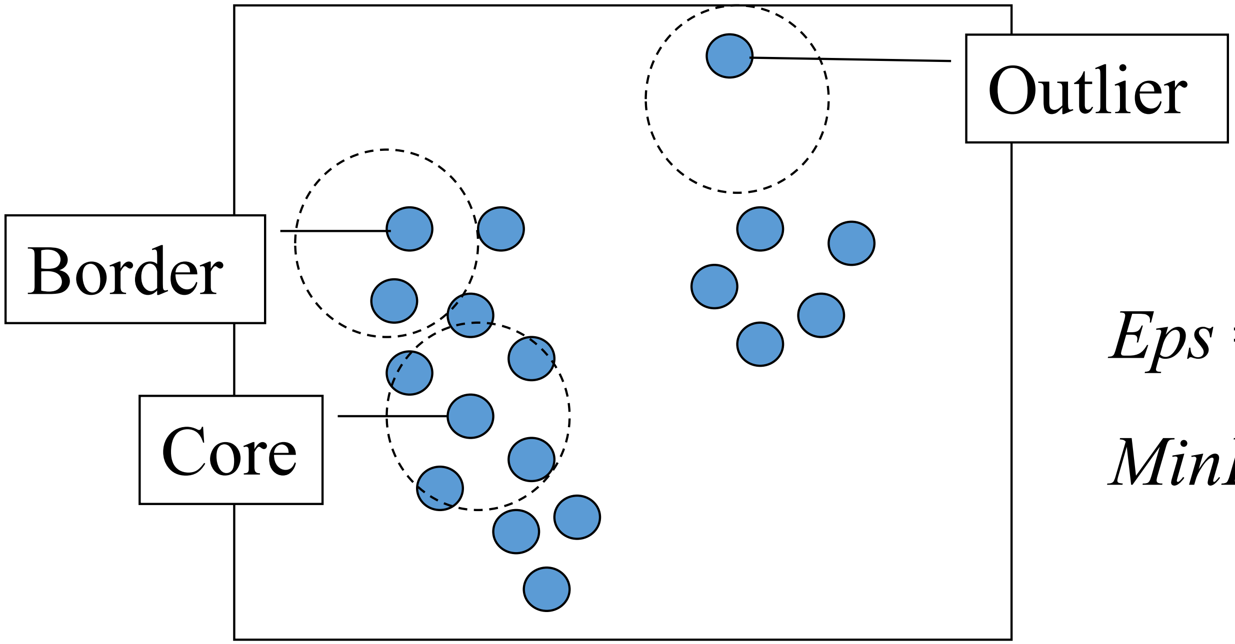
- Density-reachable:
  - A point p is density-reachable from a point q if there is a chain of points $p_1, \ldots, p_n$, $p_1 = q$, $p_n = p$ such that p_{i+1} is directly density-reachable from p_i
  - This is not symmetric



- 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



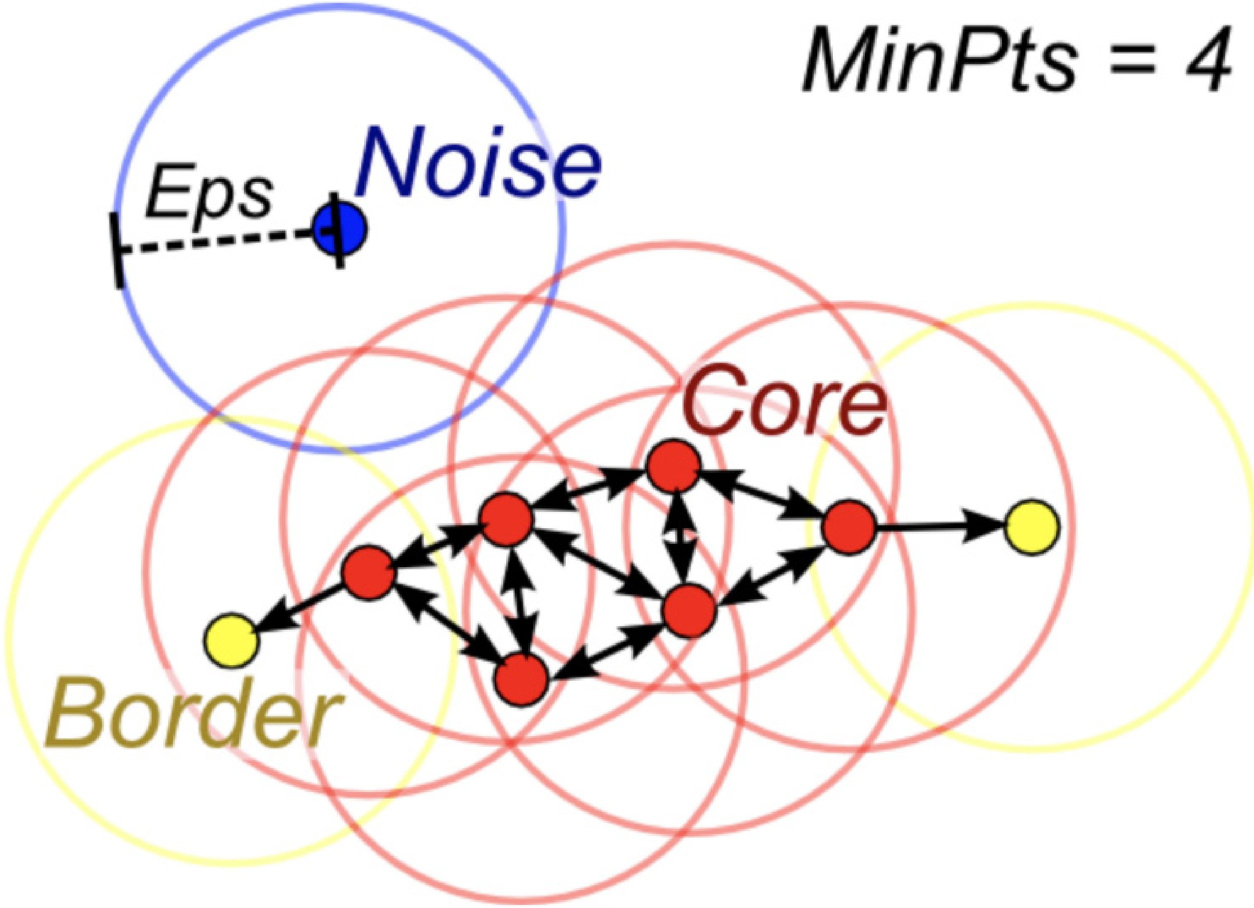
Given *Eps* and *MinPts*, categorize the objects into three exclusive groups.

$Eps = 1\text{cm}$

$MinPts = 5$

- A point is a core point if it has more than a specified number of points (*MinPts*) within *Eps*—These are points that are at the interior of a cluster.
- A border point has fewer than *MinPts* within *Eps*, but is in the neighborhood of a core point.
- A noise point is any point that is not a core point nor a border point.

DBSCAN – Core, border and noise points – Illustration - I

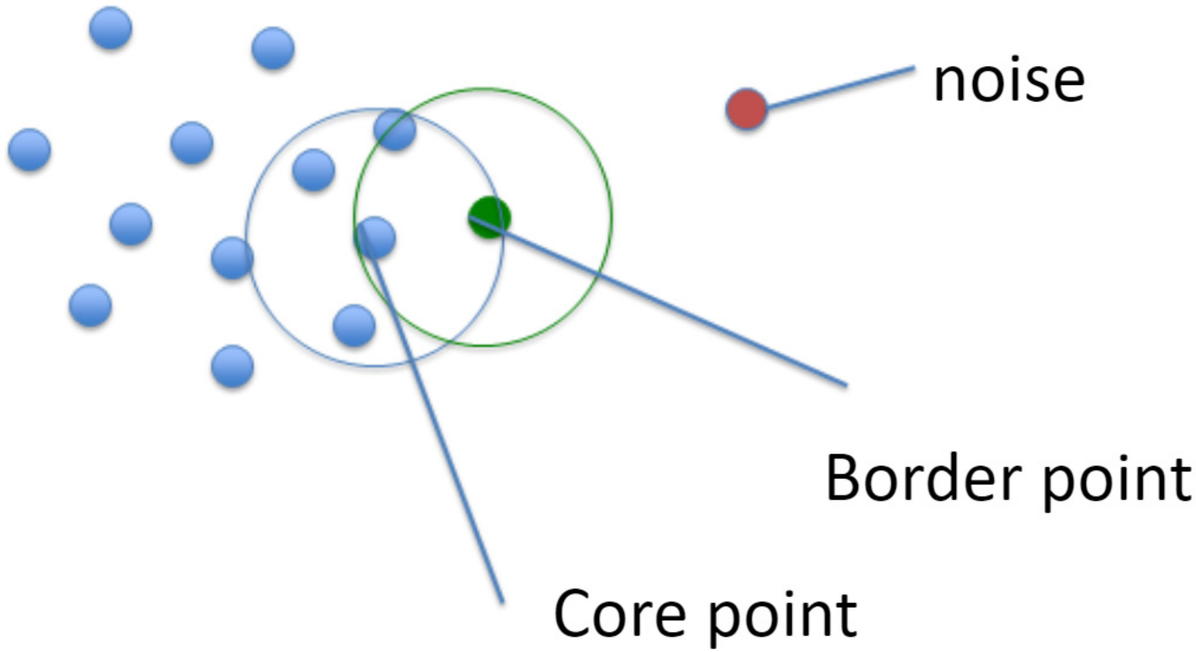


Red: Core Points

Yellow: Border points. Still part of the cluster because it's within epsilon of a core point, but not does not meet the min_points criteria

Blue: Noise point. Not assigned to a cluster

DBSCAN – Core, border and noise points – Illustration - II



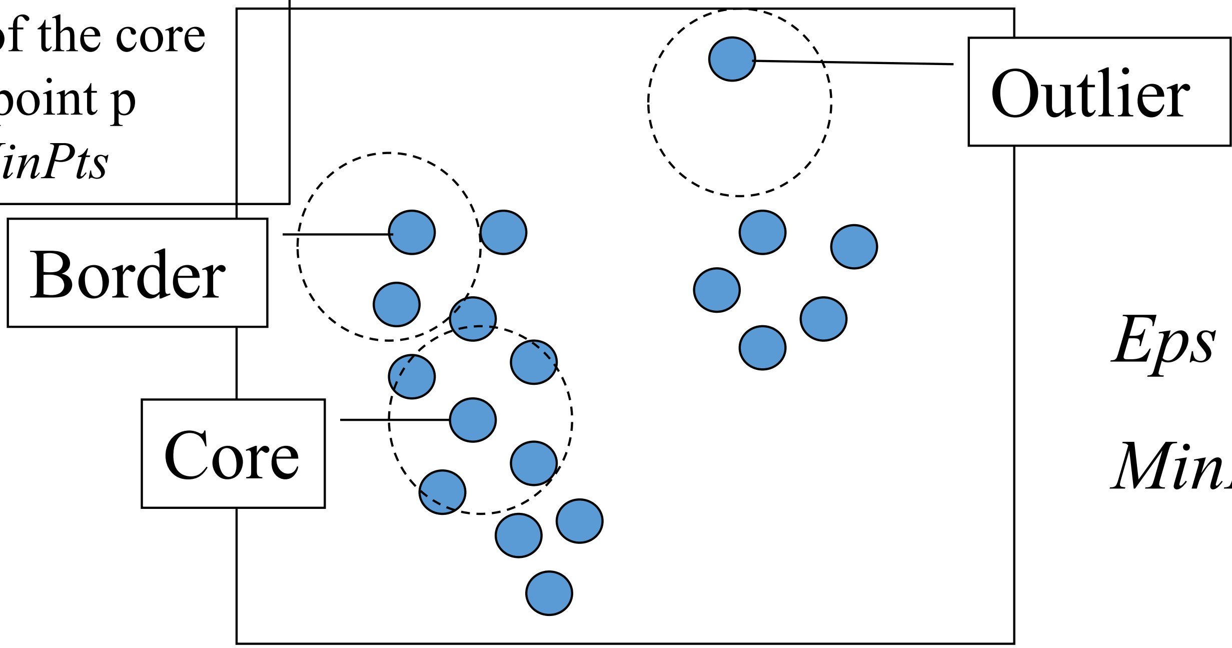
MinPts = 4

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

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

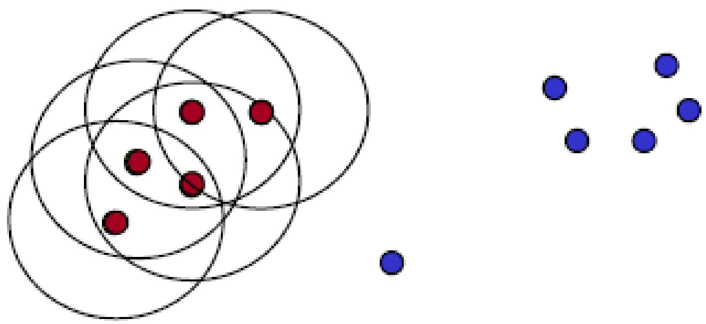


$Eps = 1\text{cm}$

$MinPts = 5$

DBSCAN Algorithm with example

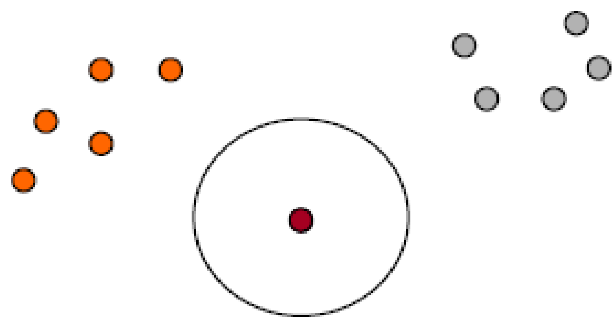
- Parameter: $\varepsilon = 2$, $MinPts = 3$



for each $o \in D$ **do**
    if o is not yet classified **then**
        if o is a core-object **then**
            collect all objects density-reachable from o
            and assign them to a new cluster.
        else
            assign o to NOISE

DBSCAN Algorithm with example

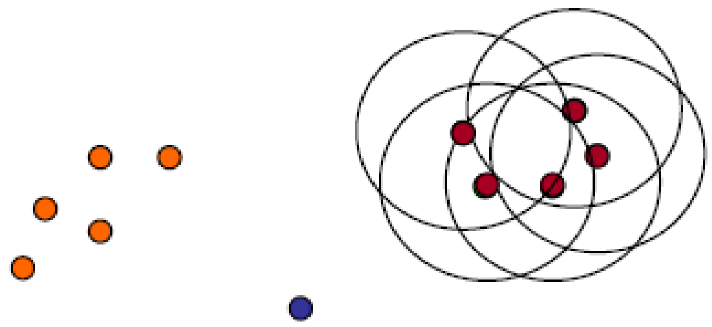
- Parameter: $\varepsilon = 2$, $MinPts = 3$



```
for each o ∈ D do
    if o is not yet classified then
        if o is a core-object then
            collect all objects density-reachable from o
            and assign them to a new cluster.
        else
            assign o to NOISE
```

DBSCAN Algorithm with example

- Parameter: ε = 2, *MinPts* = 3



```
for each o ∈ D do
    if o is not yet classified then
        if o is a core-object then
            collect all objects density-reachable from o
            and assign them to a new cluster.
        else
            assign o to NOISE
```

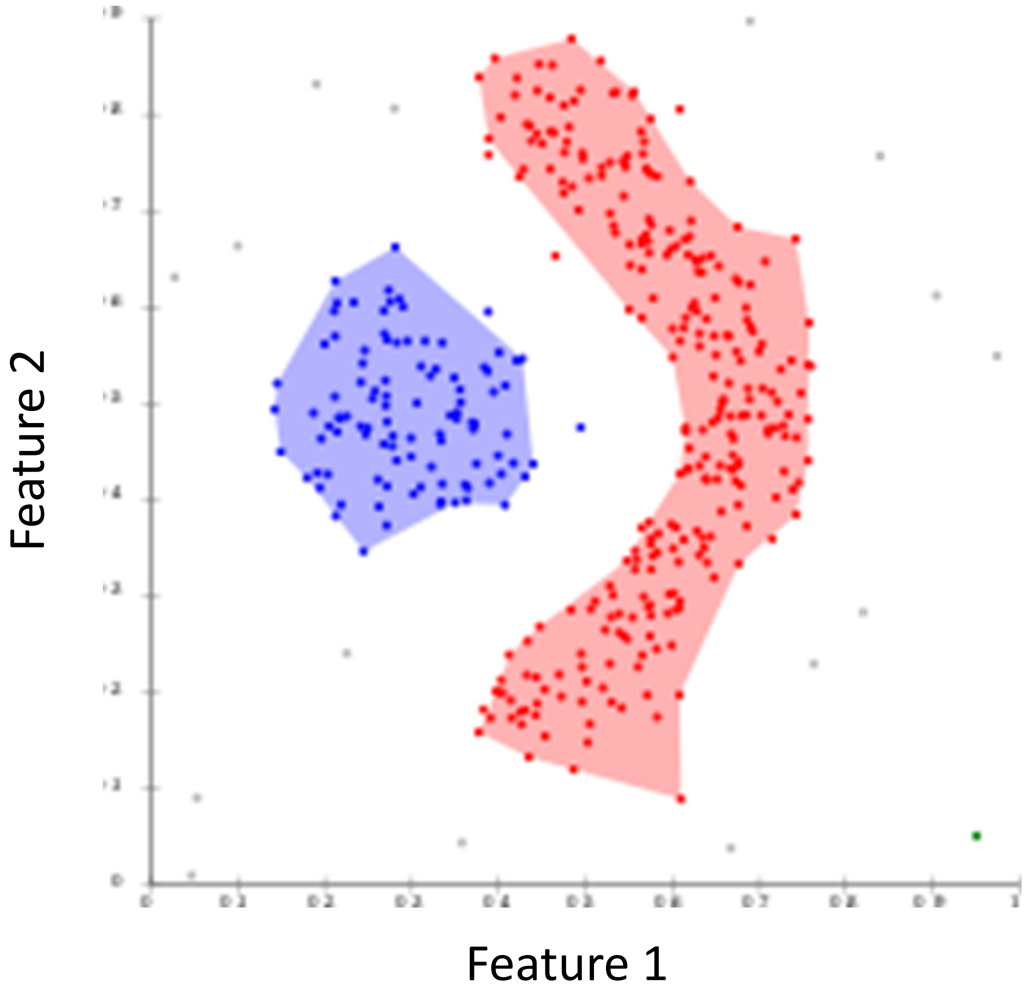
Algorithm

- **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



How to pick the initial centroids?

I'll Choose

Randomly

Farthest Point

What kind of data would you lik

Uniform Points

Gaussian Mixture

Smiley Face

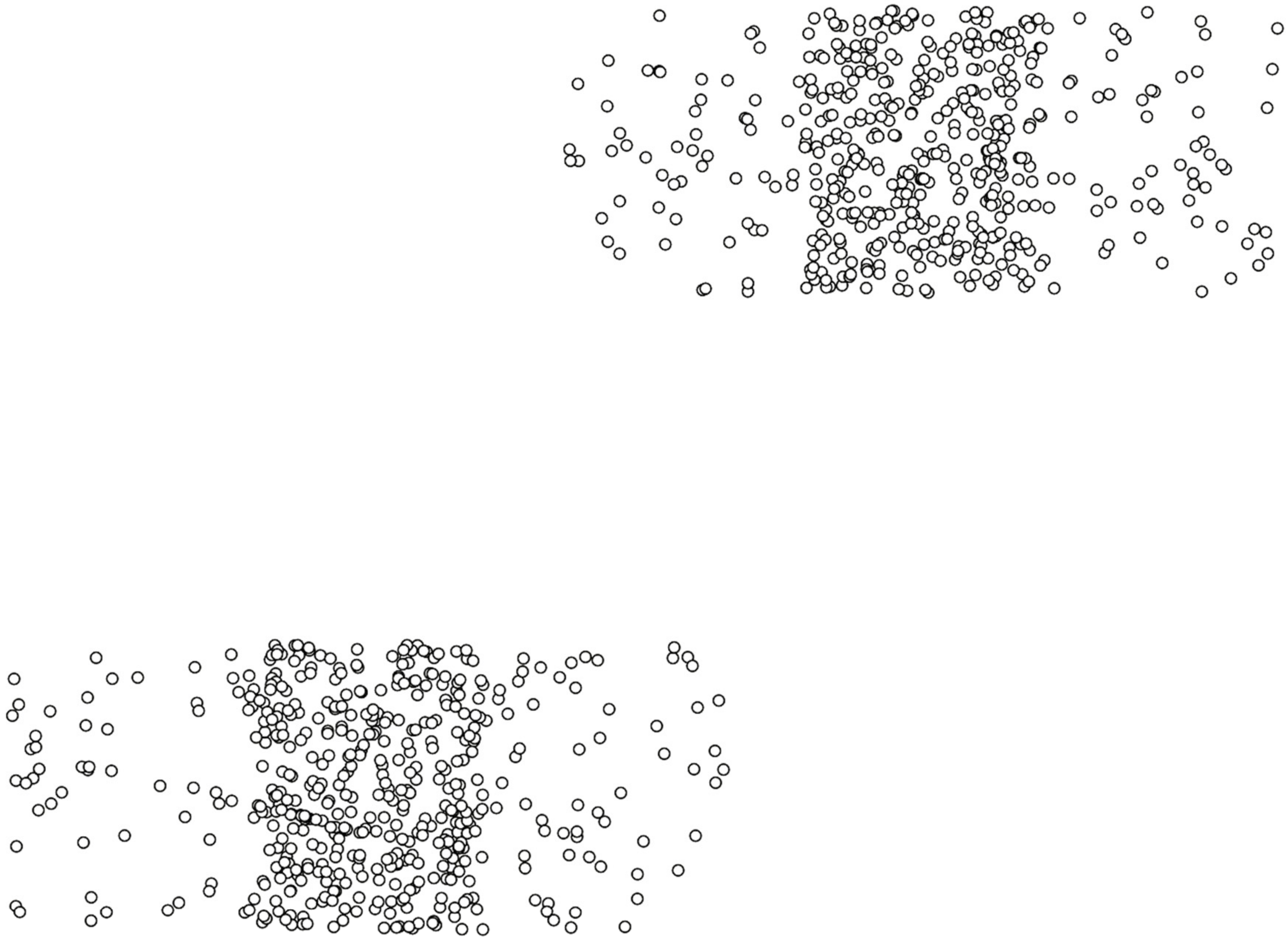
Density Bars

Packed Circles

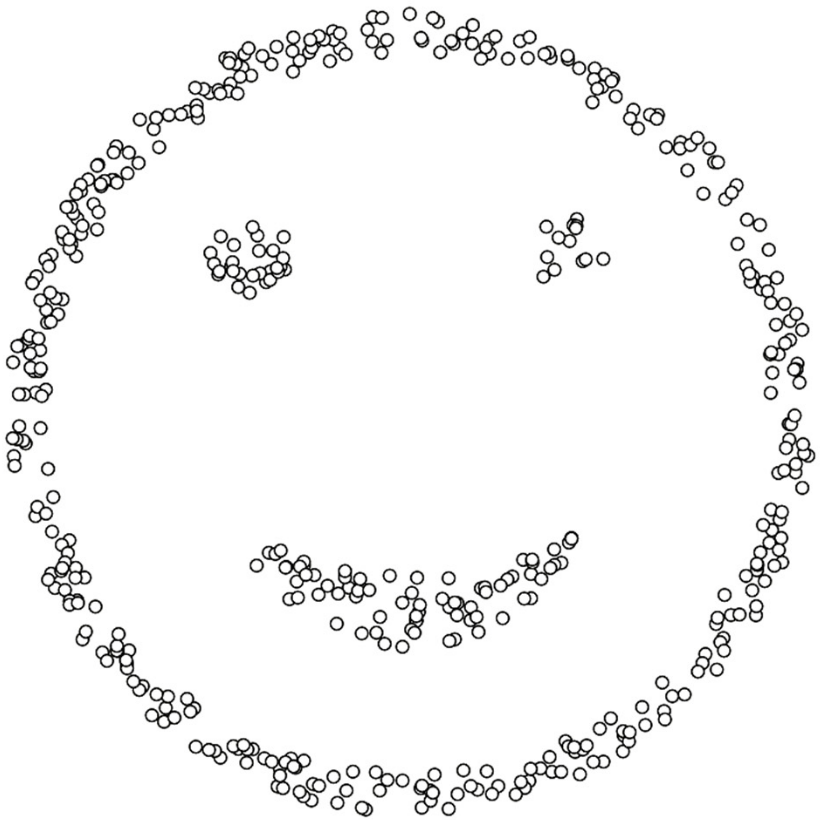
Pimpled Smil

DBSCAN Rings

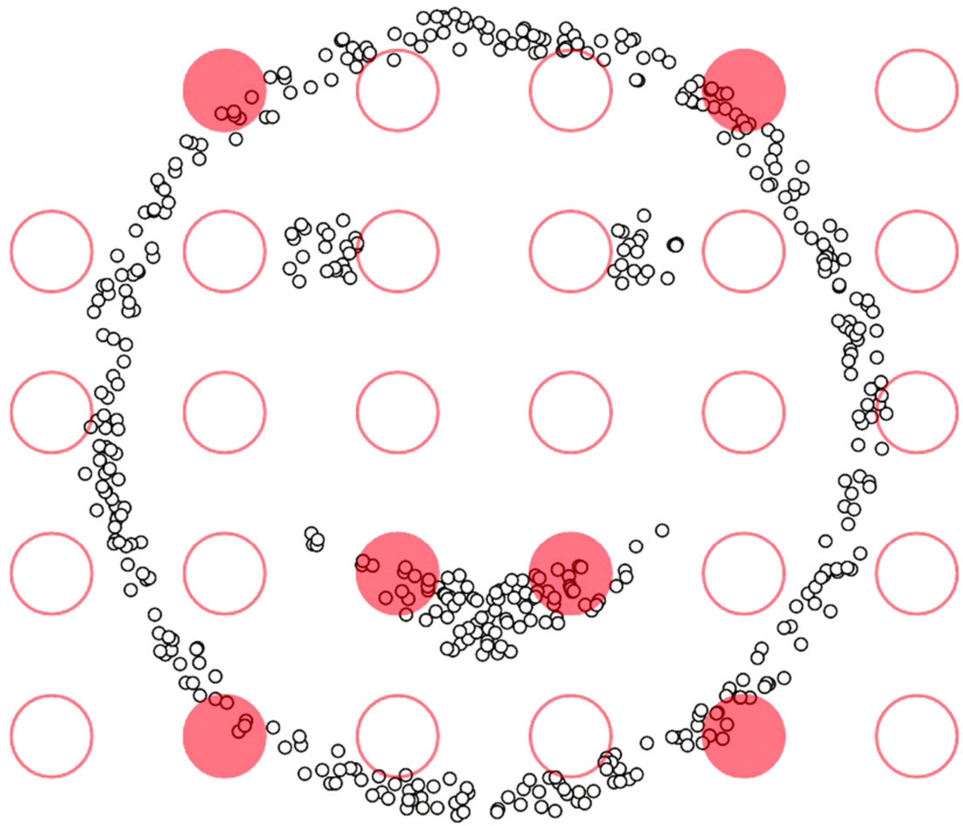
Example A

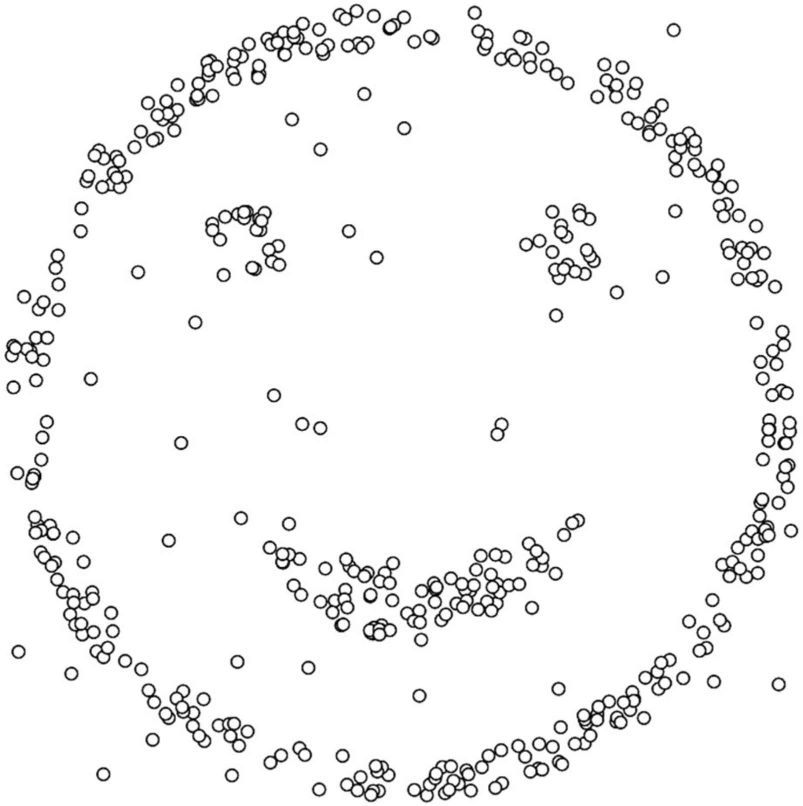


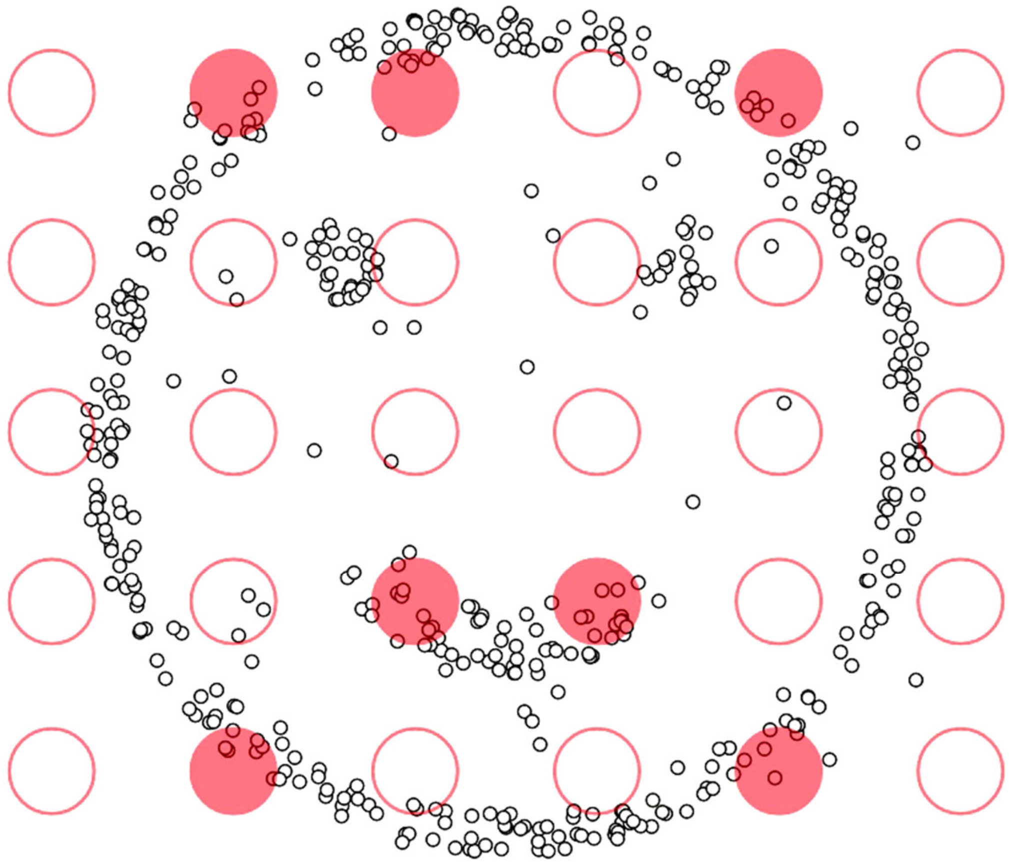
epsilon = 1.00
minPoints = 4



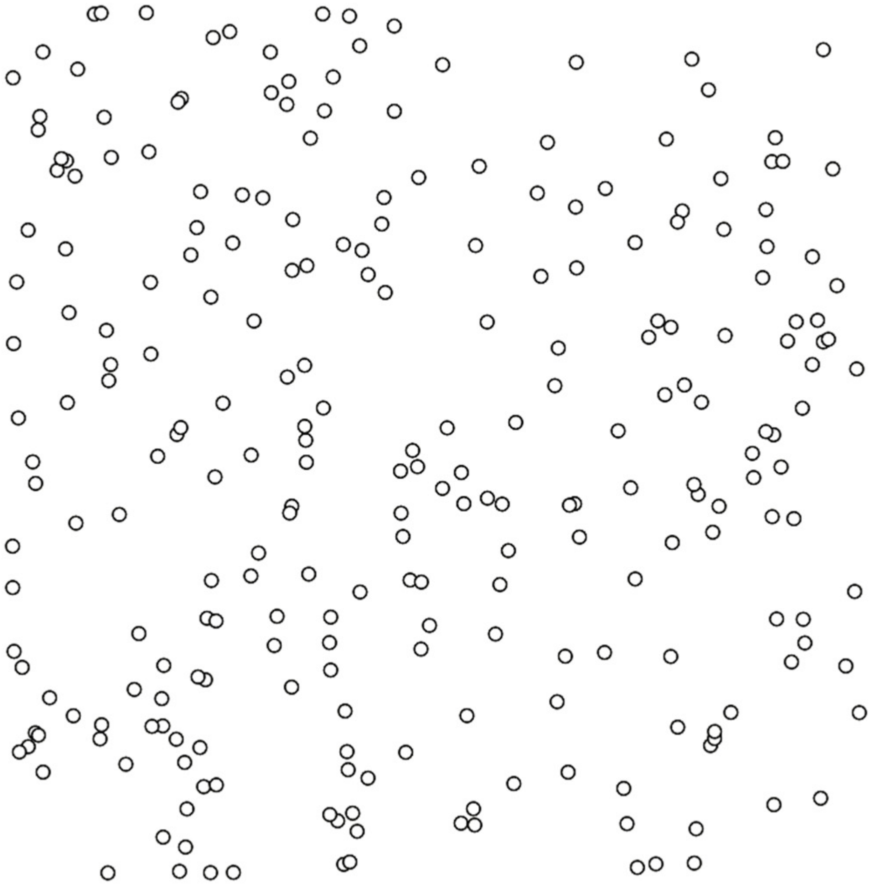
epsilon = 1.00
minPoints = 4







epsilon = 1.00
minPoints = 4



at kind of data would you like?

Uniform Points

Gaussian Mixture

Smiley Face

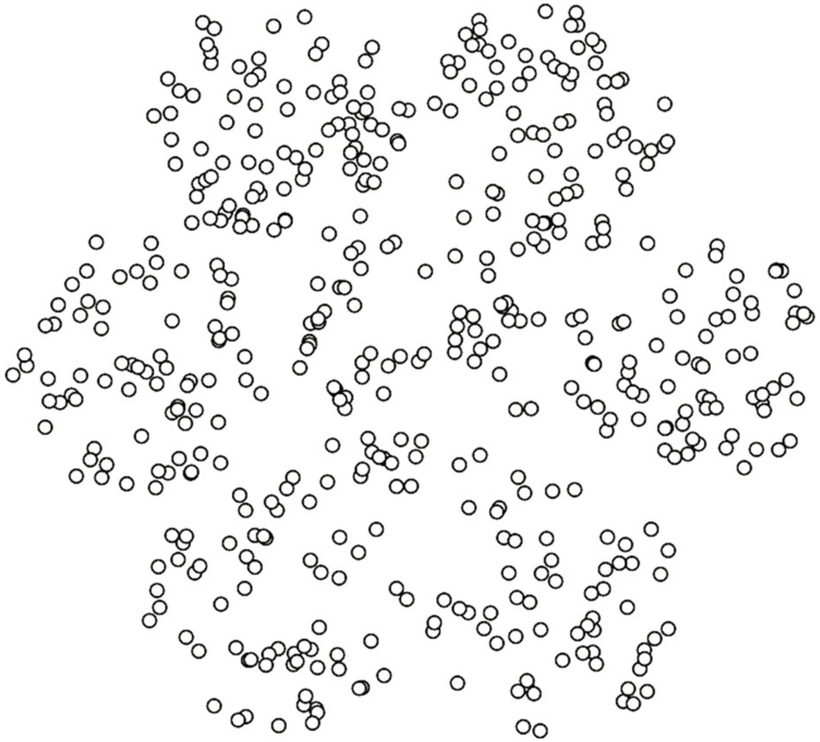
Density Bars

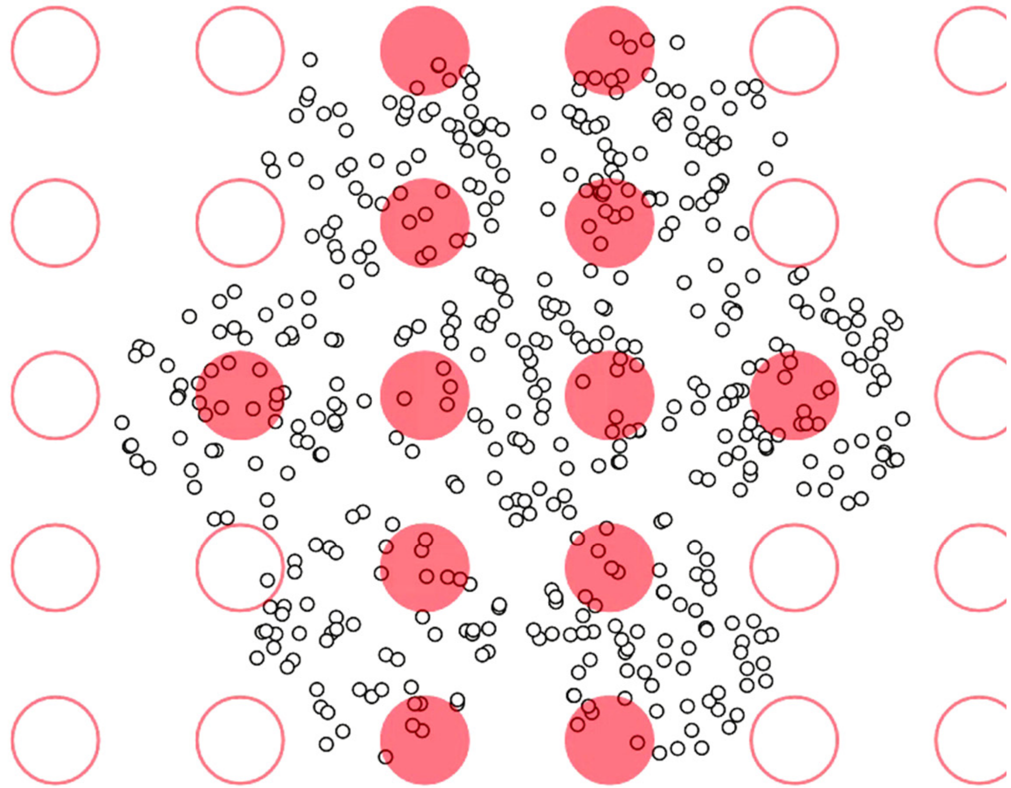
Packed Circles

Pimpled Smiley

DBSCAN Rings

Example A





epsilon = 1.00
minPoints = 4

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Demo

Visualizing DBSCAN Clustering

Link: https://www.naftaliharris.com/blog/visualizing-dbscan-clustering/

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