DATA MINING
LECTURE NOTES-1

BSc.(H) Computer Science: VI Semester

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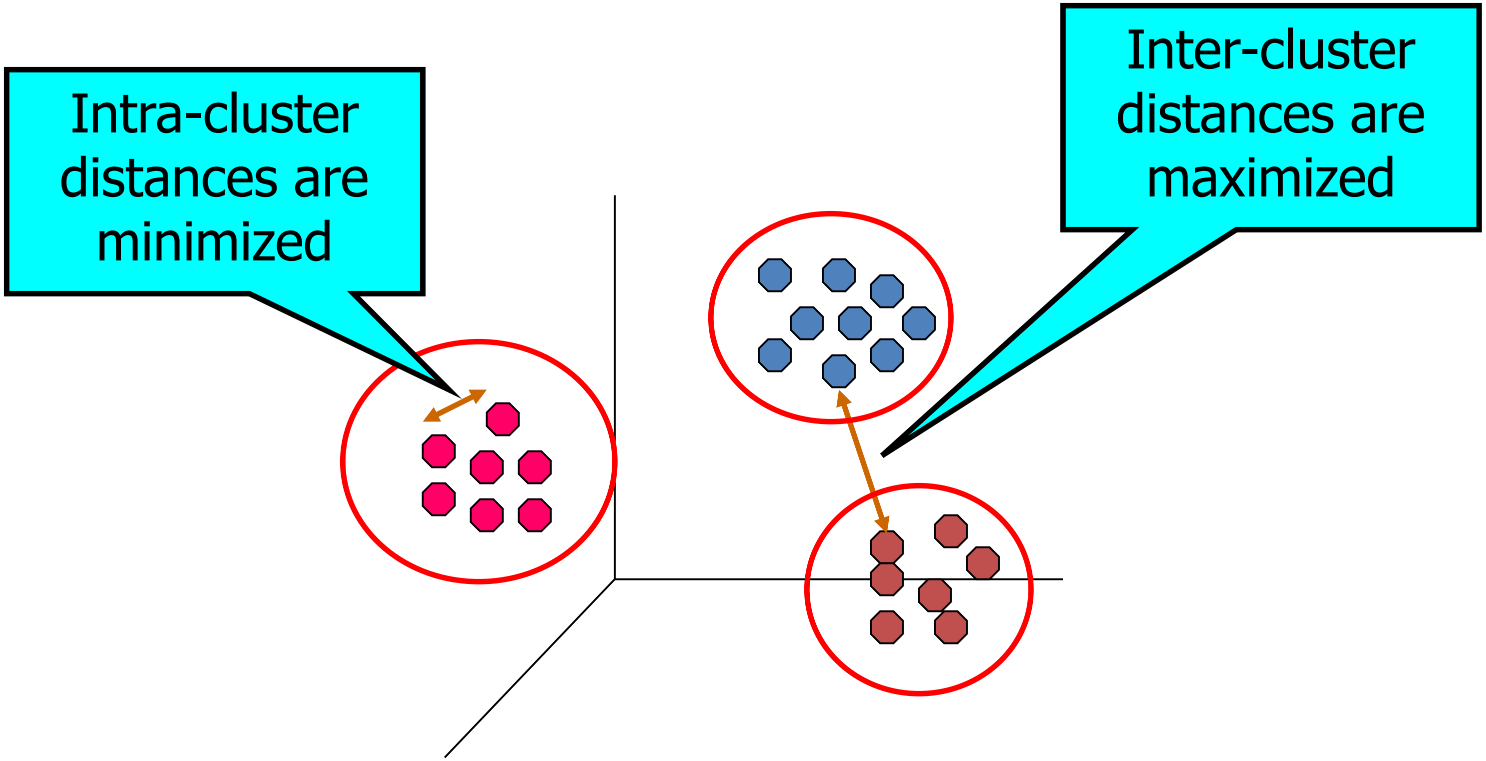
CLUSTERING

What is a Clustering?

- In general a grouping of objects such that the objects in a group (cluster) are similar (or related) to one another and different from (or unrelated to) the objects in other groups

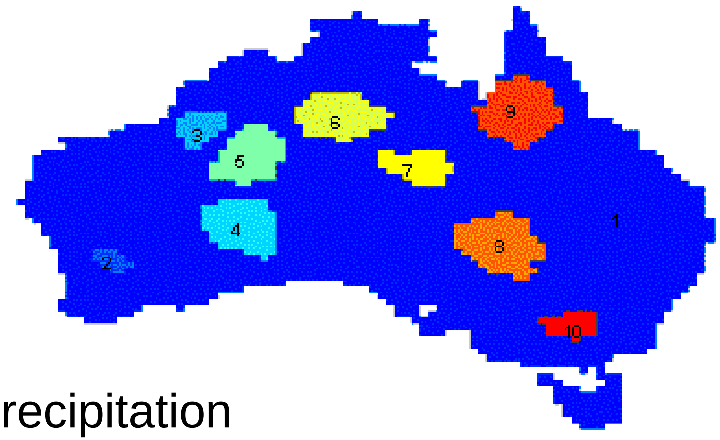


Applications of Cluster Analysis

- **Understanding**
  - Group related documents for browsing, group genes and proteins that have similar functionality, or group stocks with similar price fluctuations

	Discovered Clusters	*Industry Group*
1	Applied-Matl-DOWN,Bay-Network-Down,3-COM-DOWN, Cabletron-Sys-DOWN,CISCO-DOWN,HP-DOWN, DSC-Comm-DOWN,INTEL-DOWN,LSI-Logic-DOWN, Micron-Tech-DOWN,Texas-Inst-Down,Tellabs-Inc-Down, Natl-Semiconduct-DOWN,Oracl-DOWN,SGI-DOWN, Sun-DOWN	Technology1-DOWN
2	Apple-Comp-DOWN,Autodesk-DOWN,DEC-DOWN, ADV-Micro-Device-DOWN,Andrew-Corp-DOWN, Computer-Assoc-DOWN,Circuit-City-DOWN, Compaq-DOWN, EMC-Corp-DOWN, Gen-Inst-DOWN, Motorola-DOWN,Microsoft-DOWN,Scientific-Atl-DOWN	Technology2-DOWN
3	Fannie-Mae-DOWN,Fed-Home-Loan-DOWN, MBNA-Corp-DOWN,Morgan-Stanley-DOWN	Financial-DOWN
4	Baker-Hughes-UP,Dresser-Inds-UP,Halliburton-HLD-UP, Louisiana-Land-UP,Phillips-Petro-UP,Unocal-UP, Schlumberger-UP	Oil-UP

- **Summarization**
  - Reduce the size of large data sets



Clustering precipitation in Australia

Early applications of cluster analysis

- John Snow, London 1854

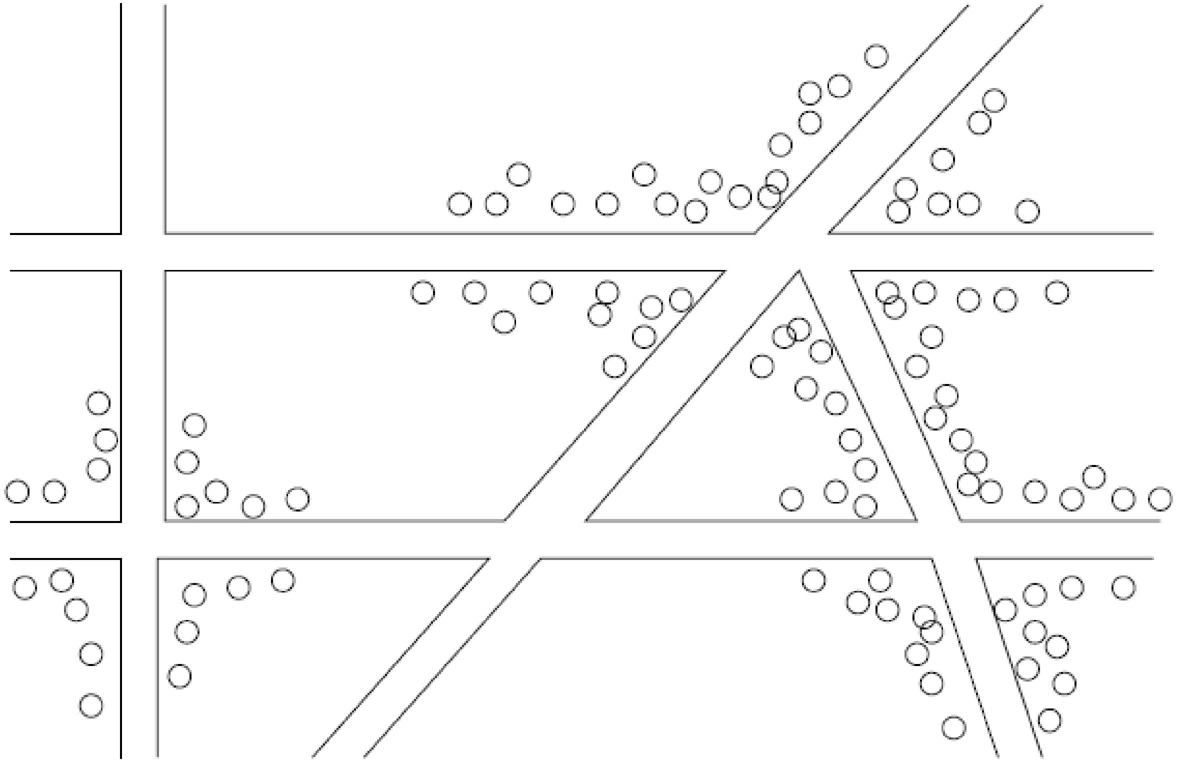
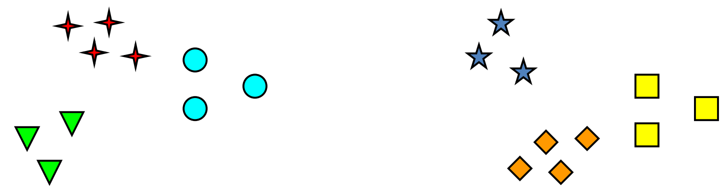


Figure 1.1: Plotting cholera cases on a map of London

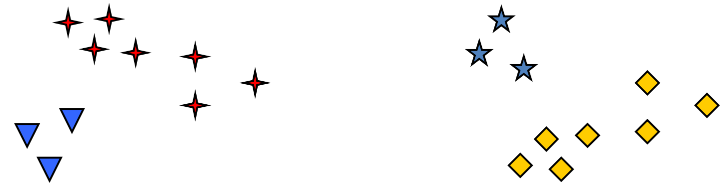
Notion of a Cluster can be Ambiguous

How many clusters?



Six Clusters

Two Clusters

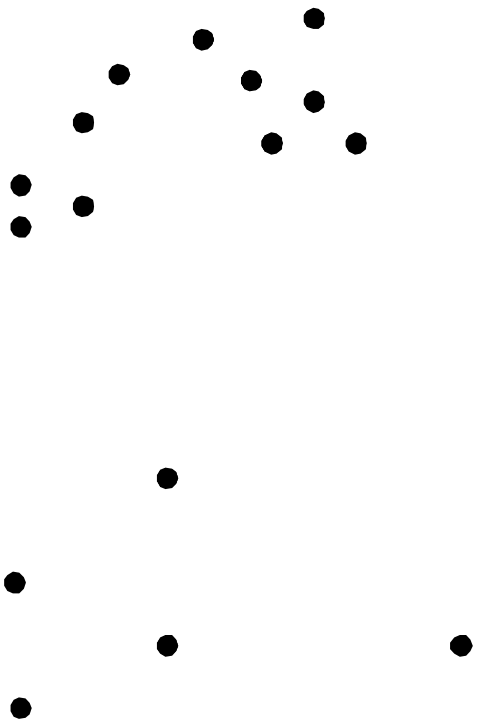


Four Clusters

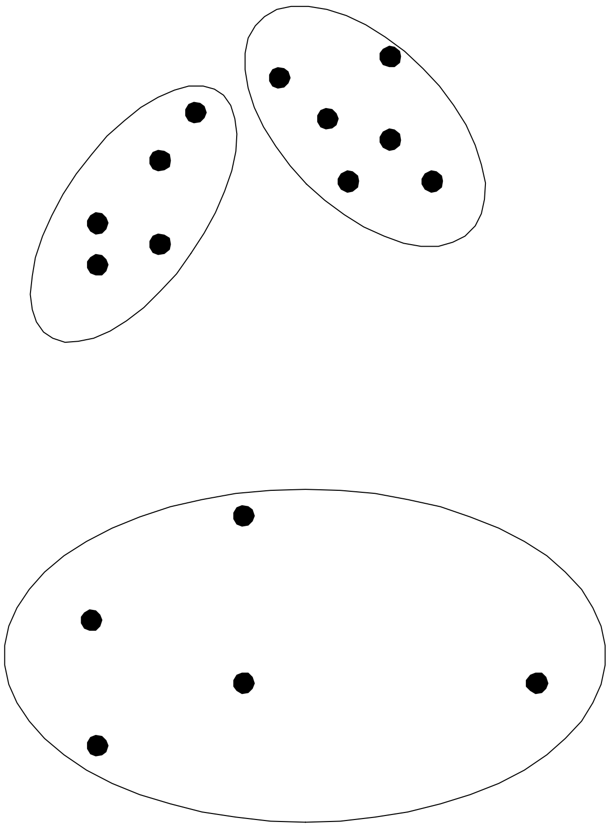
Types of Clusterings

- A clustering is a set of clusters
- Important distinction between hierarchical and partitional sets of clusters
- Partitional Clustering
  - A division data objects into subsets (clusters) such that each data object is in exactly one subset
- Hierarchical clustering
  - A set of nested clusters organized as a hierarchical tree

Partitional Clustering

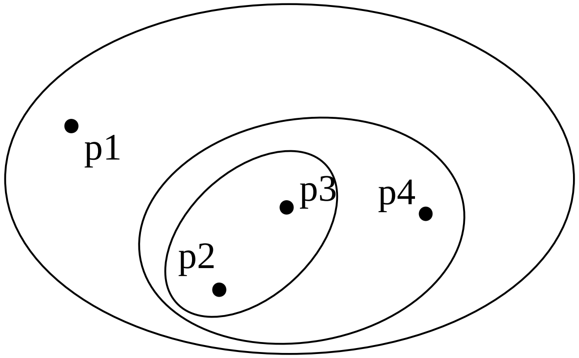


Original Points

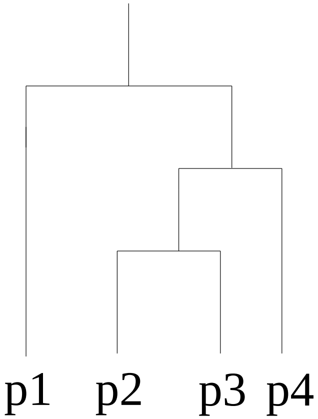


A Partitional Clustering

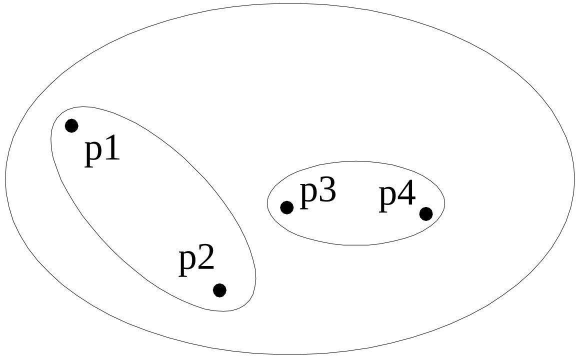
Hierarchical Clustering



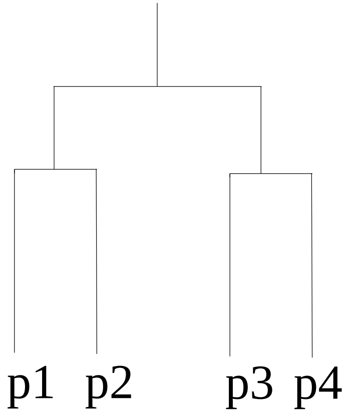
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering



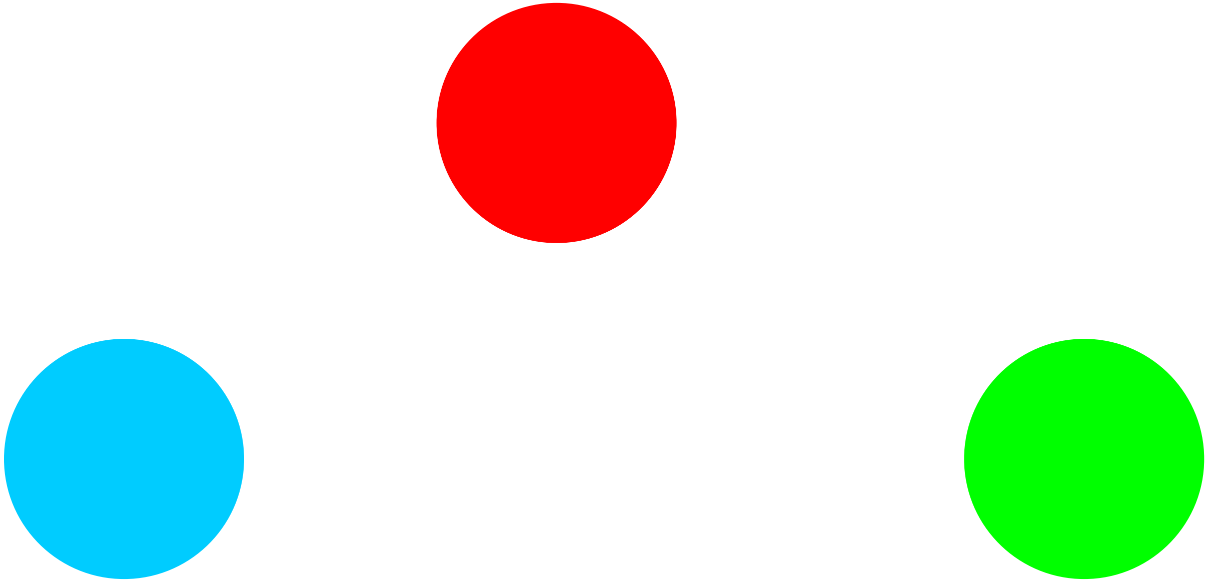
Non-traditional Dendrogram

Other types of clustering

- Exclusive (or non-overlapping) versus non-exclusive (or overlapping)
  - In non-exclusive clusterings, points may belong to multiple clusters.
    - Points that belong to multiple classes, or ‘border’ points
- Fuzzy (or soft) versus non-fuzzy (or hard)
  - In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1
    - Weights usually must sum to 1 (often interpreted as probabilities)
- Partial versus complete
  - In some cases, we only want to cluster some of the data

Types of Clusters: Well-Separated

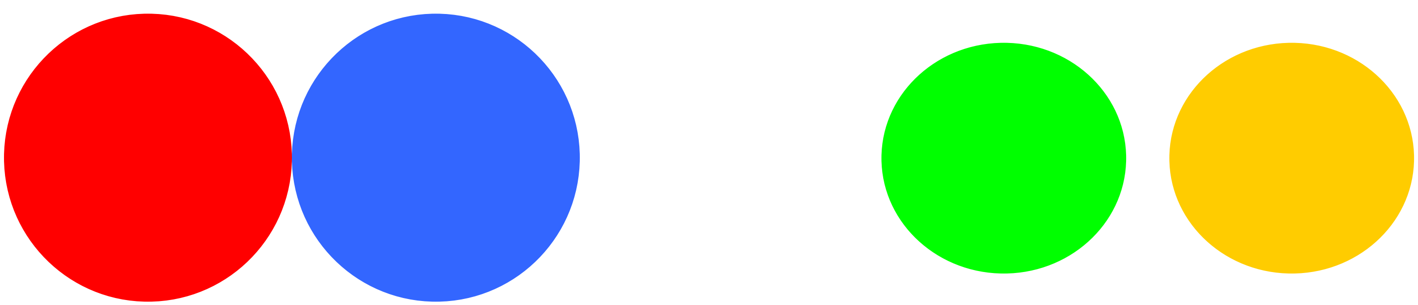
- Well-Separated Clusters:
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.



3 well-separated clusters

Types of Clusters: Center-Based

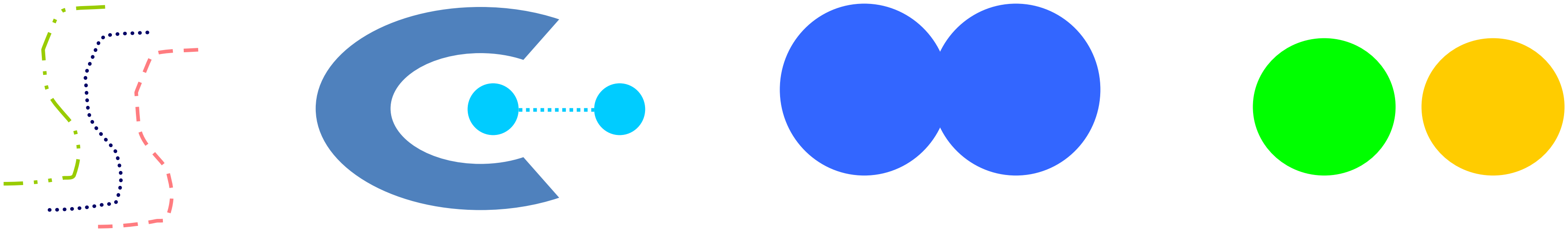
- Center-based
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the "center" of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the minimizer of distances from all the points in the cluster, or a medoid, the most "representative" point of a cluster



4 center-based clusters

Types of Clusters: Contiguity-Based

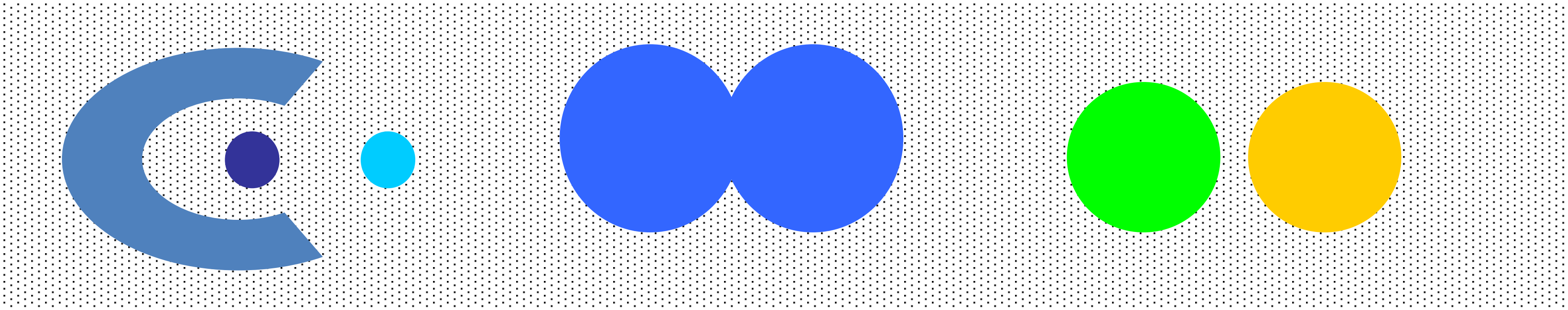
- Contiguous Cluster (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.



8 contiguous clusters

Types of Clusters: Density-Based

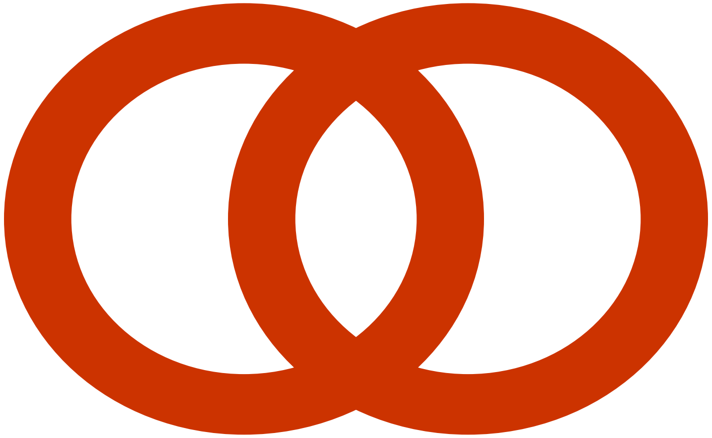
- Density-based
  - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
  - Used when the clusters are irregular or intertwined, and when noise and outliers are present.



6 density-based clusters

Types of Clusters: Conceptual Clusters

- Shared Property or Conceptual Clusters
  - Finds clusters that share some common property or represent a particular concept.
  - .



2 Overlapping Circles

Types of Clusters: Objective Function

- Clustering as an optimization problem
  - Finds clusters that minimize or maximize an objective function.
  - Enumerate all possible ways of dividing the points into clusters and evaluate the `goodness' of each potential set of clusters by using the given objective function. (NP Hard)
  - Can have global or local objectives.
    - Hierarchical clustering algorithms typically have local objectives
    - Partitional algorithms typically have global objectives
  - A variation of the global objective function approach is to fit the data to a parameterized model.
    - The parameters for the model are determined from the data, and they determine the clustering
    - E.g., Mixture models assume that the data is a ‘mixture' of a number of statistical distributions.

Clustering Algorithms

- K-means and its variants
- Hierarchical clustering
- DBSCAN

K-MEANS

K-means Clustering

- Partitional clustering approach
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid
- Number of clusters, K, must be specified
- The objective is to minimize the sum of distances of the points to their respective centroid

K-means Clustering

- **Problem:** Given a set X of n points in a d-dimensional space and an integer K group the points into K clusters $C = \{C_1, C_2, \ldots, C_k\}$ such that

$$Cost(C) = \sum_{i=1}^{k} \sum_{x \in C_i} dist(x, c)$$

is minimized, where c_i is the centroid of the points in cluster C_i

K-means Clustering

- Most common definition is with euclidean distance, minimizing the Sum of Squares Error (SSE) function
  - Sometimes K-means is defined like that

- **Problem:** Given a set X of n points in a d-dimensional space and an integer K group the points into K clusters $C = \{C_1, C_2, \ldots, C_k\}$ such that

$$Cost(C) = \sum_{i=1}^{k} \sum_{x \in C_i} (x - c_i)^2$$

is minimized, where c_i is the mean of the points in cluster C_i

Sum of Squares Error (SSE)

Complexity of the k-means problem

- NP-hard if the dimensionality of the data is at least 2 (**d>=2**)
  - Finding the best solution in polynomial time is infeasible

- For **d=1** the problem is solvable in polynomial time (how?)

- A simple iterative algorithm works quite well in practice

K-means Algorithm

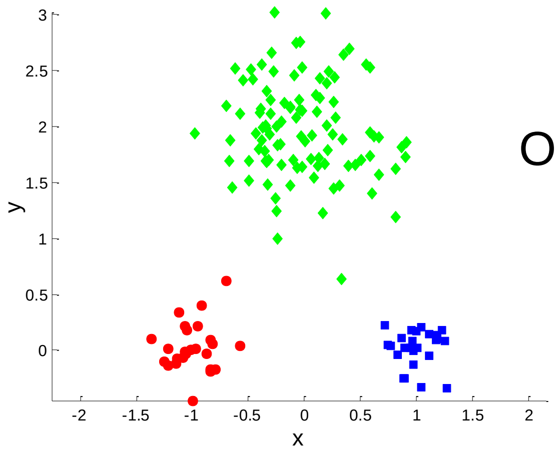
- Also known as Lloyd's algorithm.
- K-means is sometimes synonymous with this algorithm

```
Select K points as the initial centroids.
repeat
    Form K clusters by assigning all points to the closest centroid.
    Recompute the centroid of each cluster.
until The centroids don't change
```

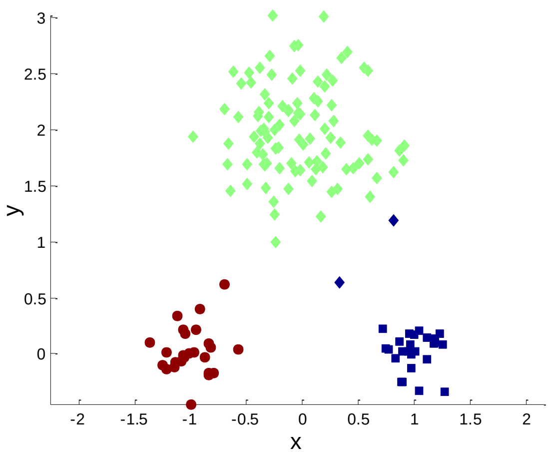
K-means Algorithm – Initialization

- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.

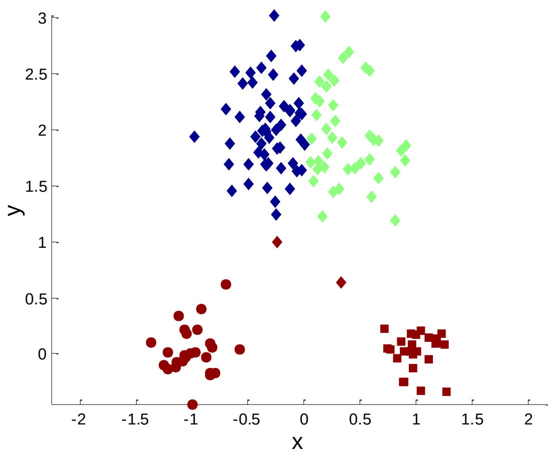
Two different K-means Clusterings



Original Points

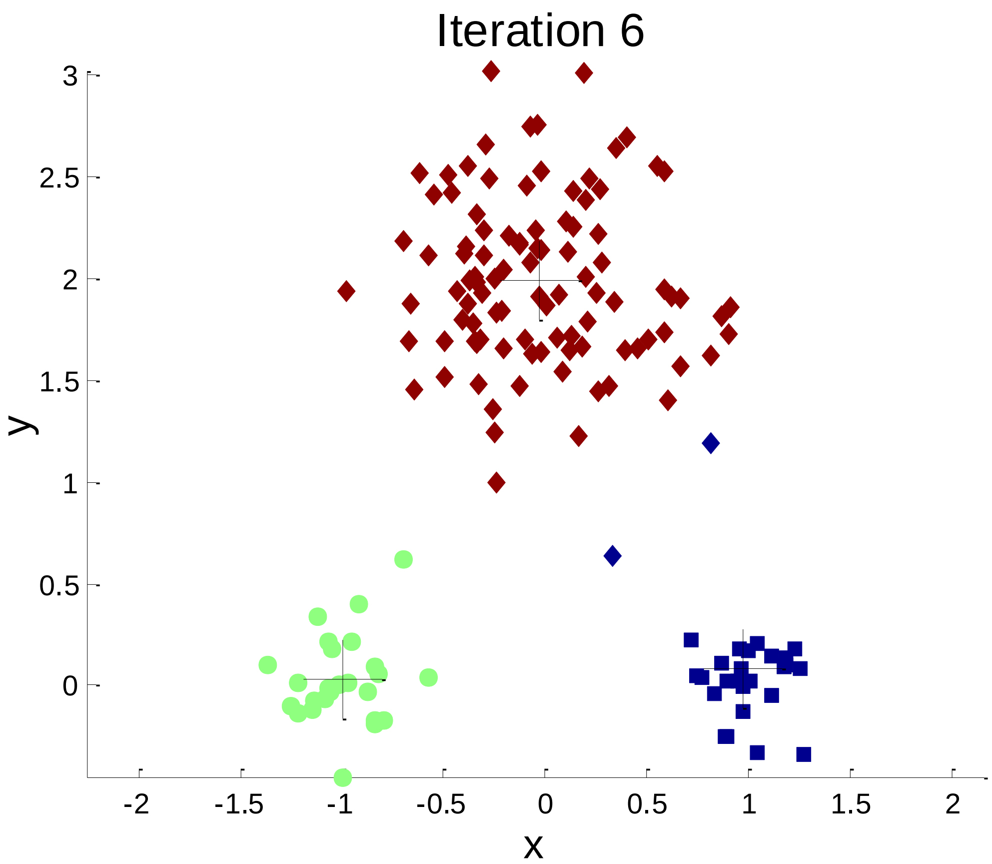


Optimal Clustering

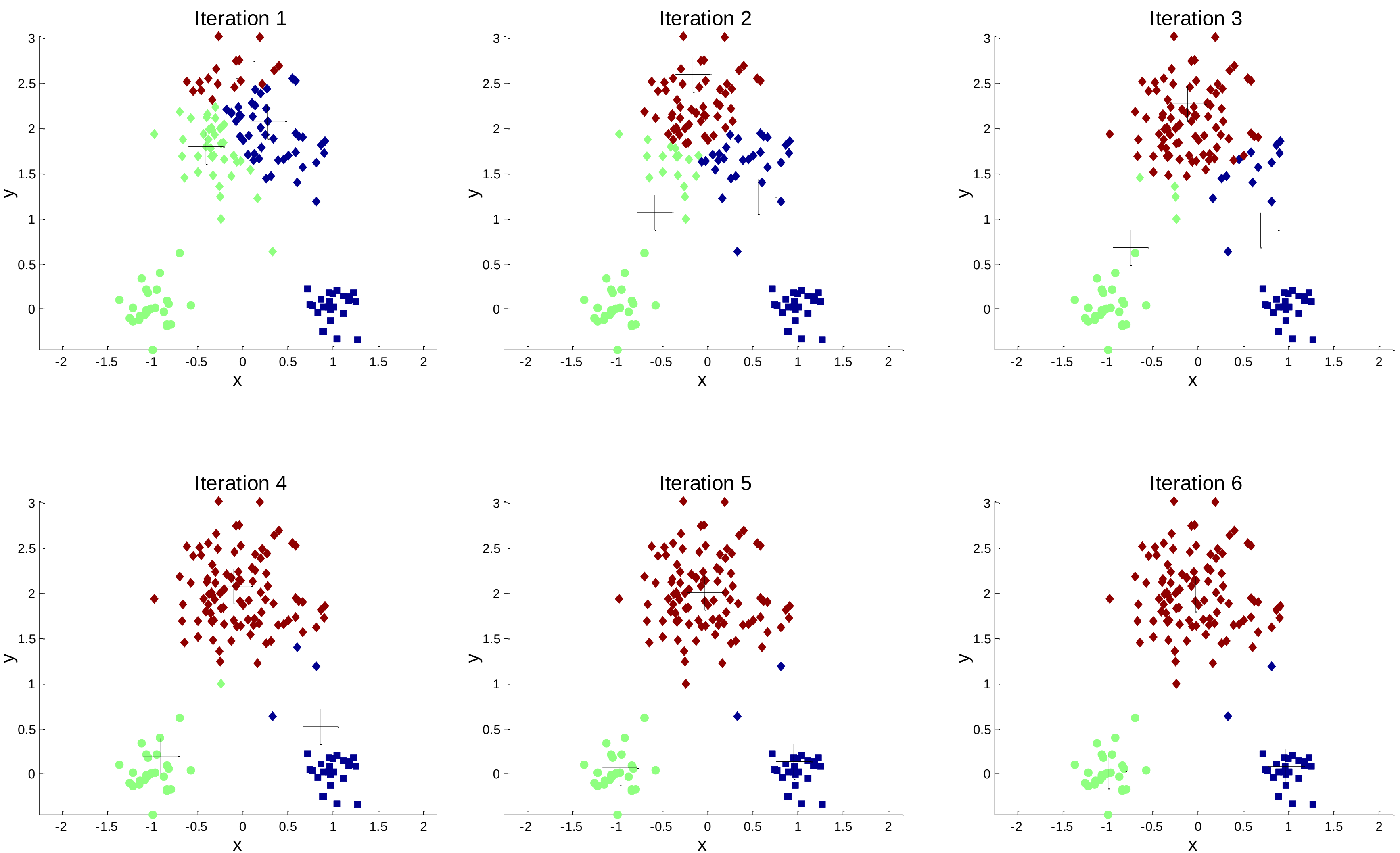


Sub-optimal Clustering

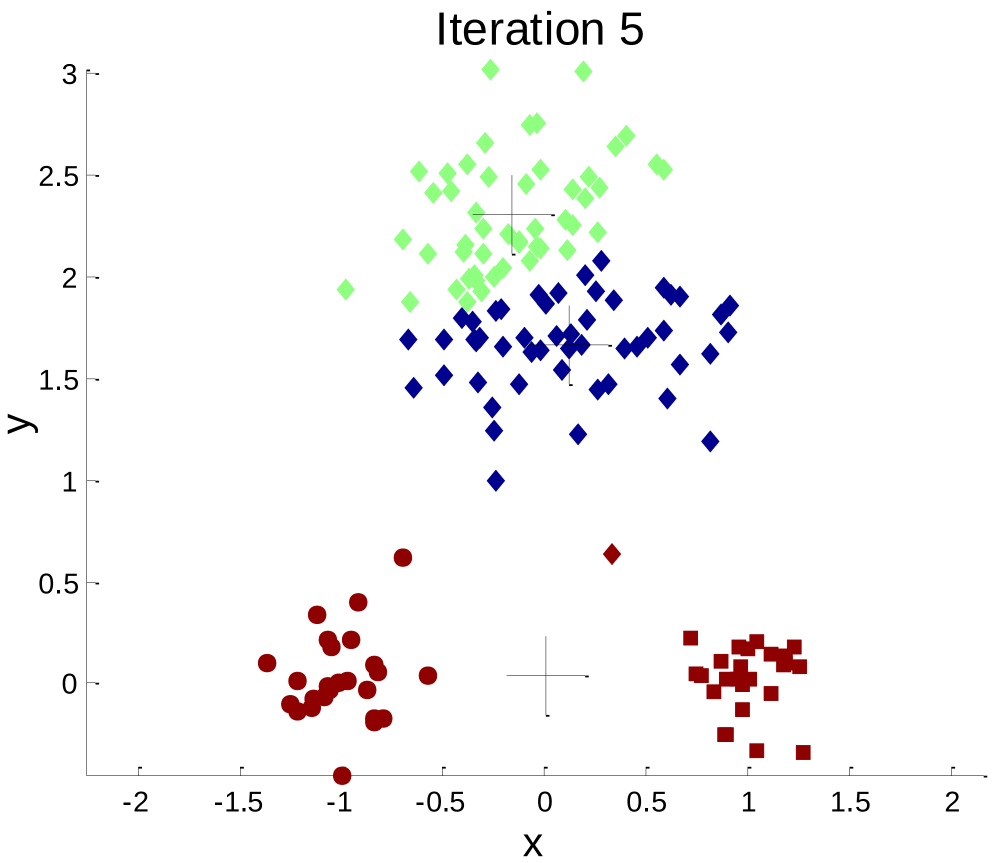
Importance of Choosing Initial Centroids



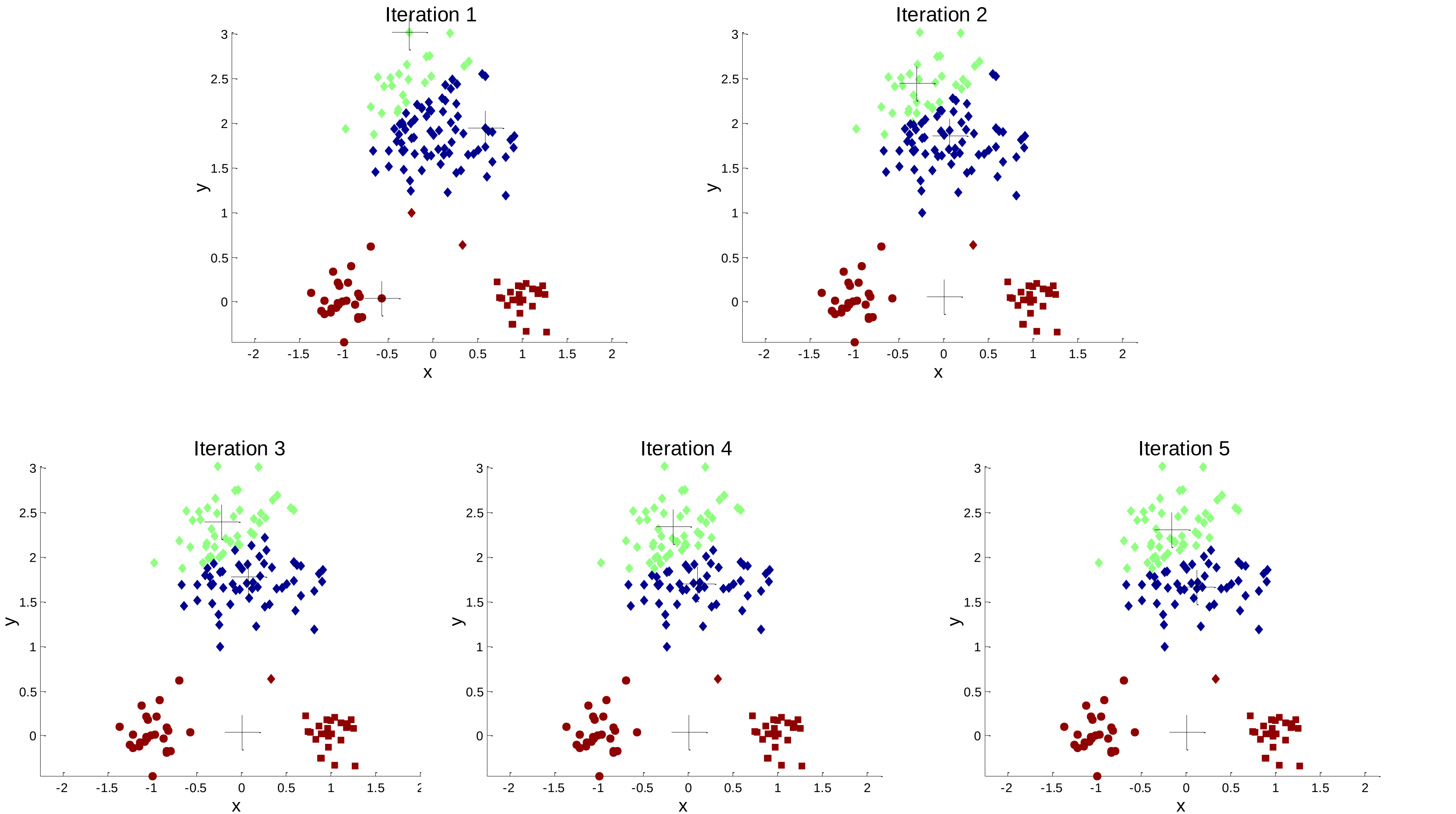
Importance of Choosing Initial Centroids



Importance of Choosing Initial Centroids



Importance of Choosing Initial Centroids …



Dealing with Initialization

- Do multiple runs and select the clustering with the smallest error

- Select original set of points by methods other than random . E.g., pick the most distant (from each other) points as cluster centers (K-means++ algorithm)

K-means Algorithm – Centroids

- The centroid depends on the distance function
  - The minimizer for the distance function
- 'Closeness' is measured by Euclidean distance (SSE), cosine similarity, correlation, etc.
- Centroid:
  - The mean of the points in the cluster for SSE, and cosine similarity
  - The median for Manhattan distance.

- Finding the centroid is not always easy
  - It can be an NP-hard problem for some distance functions
    - E.g., median form multiple dimensions

K-means Algorithm – Convergence

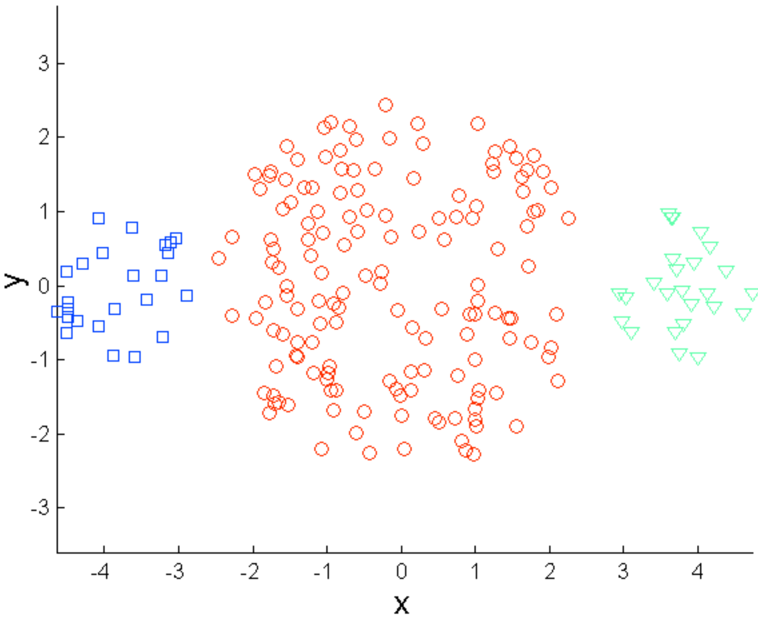
- K-means will converge for common similarity measures mentioned above.
  - Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to ‘Until relatively few points change clusters’
- Complexity is O(n * K * I * d)
  - n = number of points, K = number of clusters,
    I = number of iterations, d = dimensionality
- In general a fast and efficient algorithm

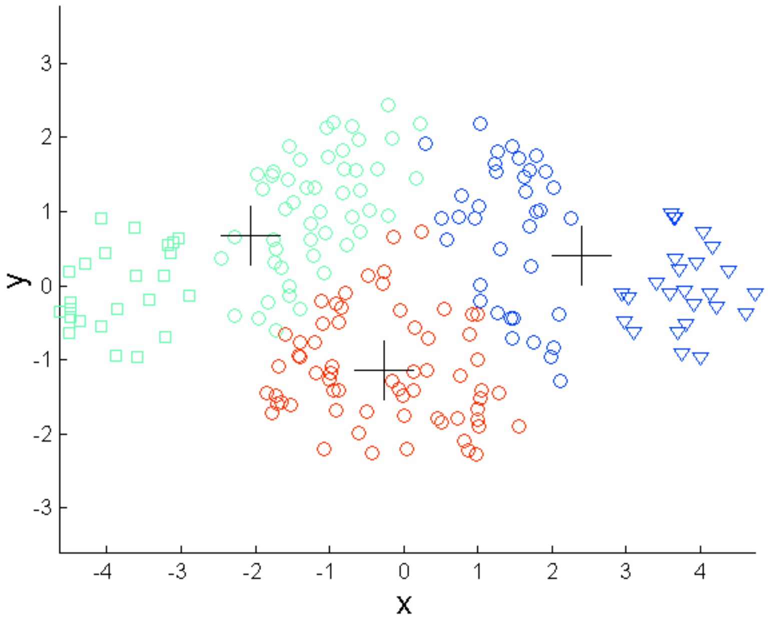
Limitations of K-means

- K-means has problems when clusters are of different
  - Sizes
  - Densities
  - Non-globular shapes

- K-means has problems when the data contains outliers.

Limitations of K-means: Differing Sizes

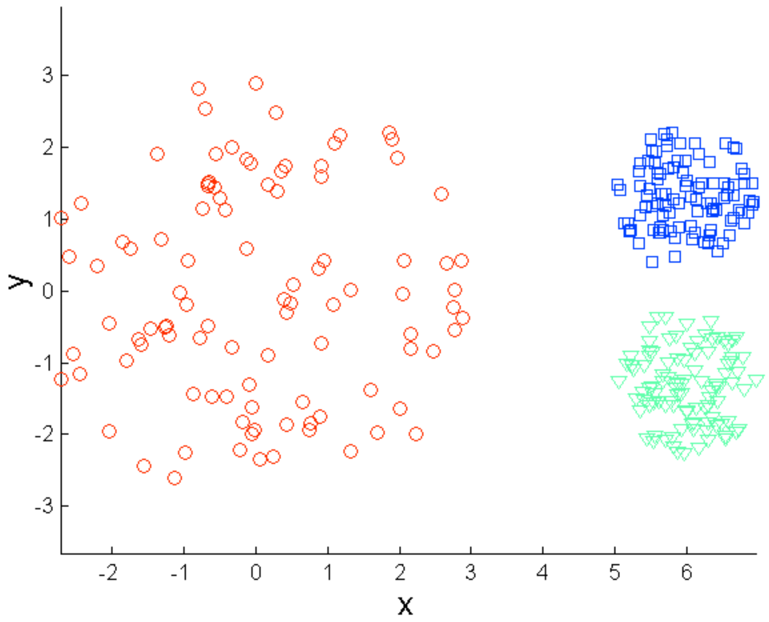




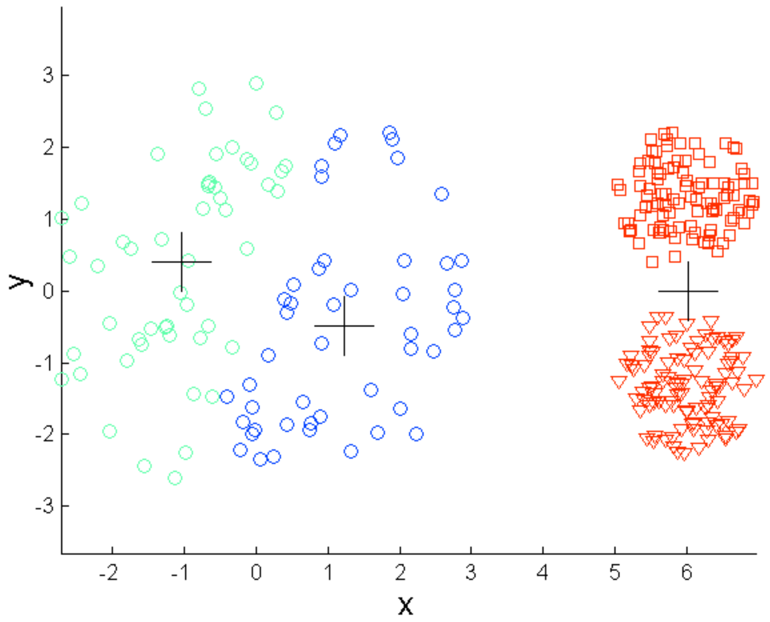
Original Points

K-means (3 Clusters)

Limitations of K-means: Differing Density

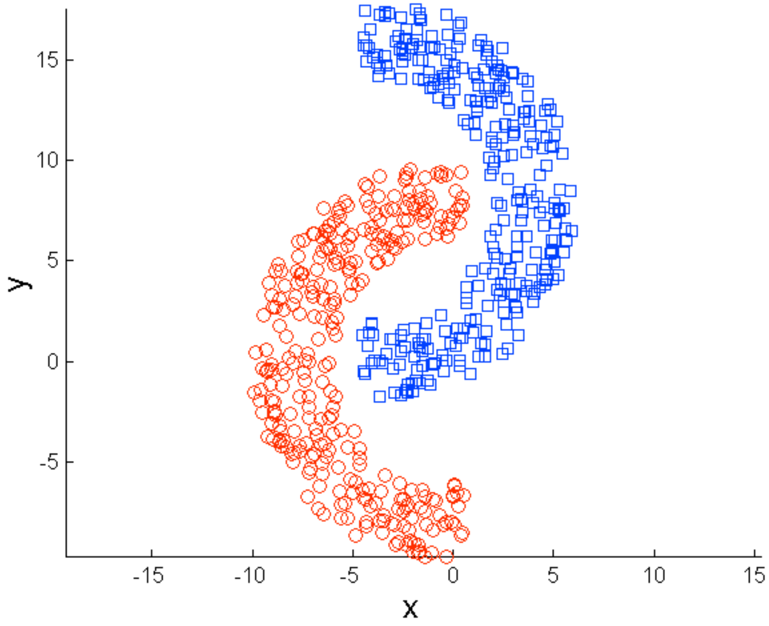


Original Points

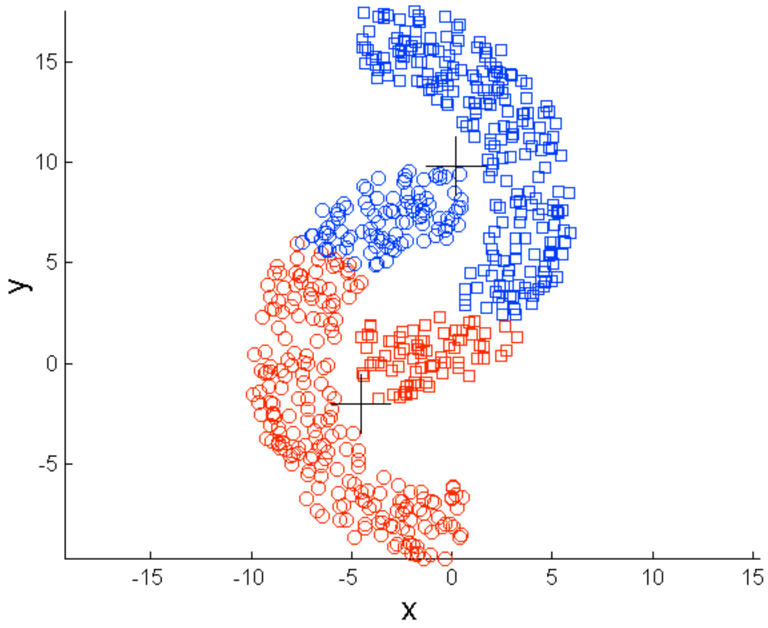


K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes

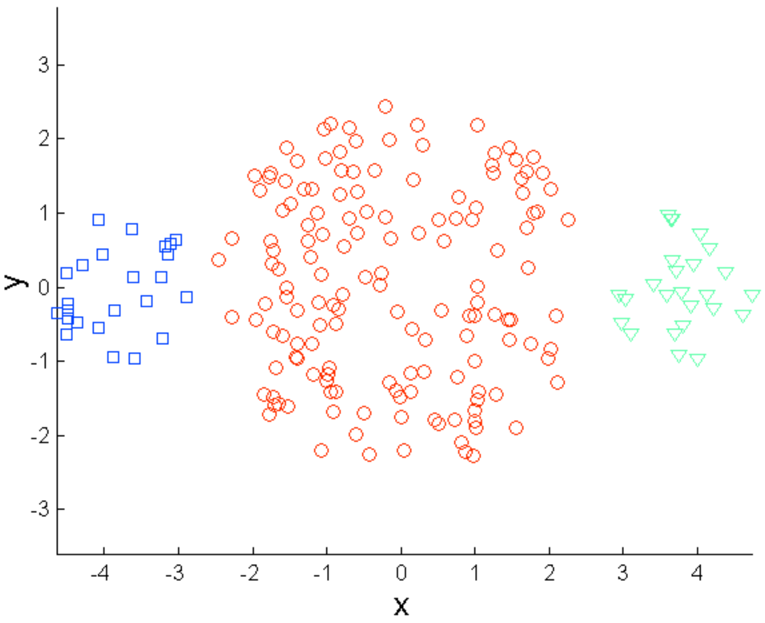


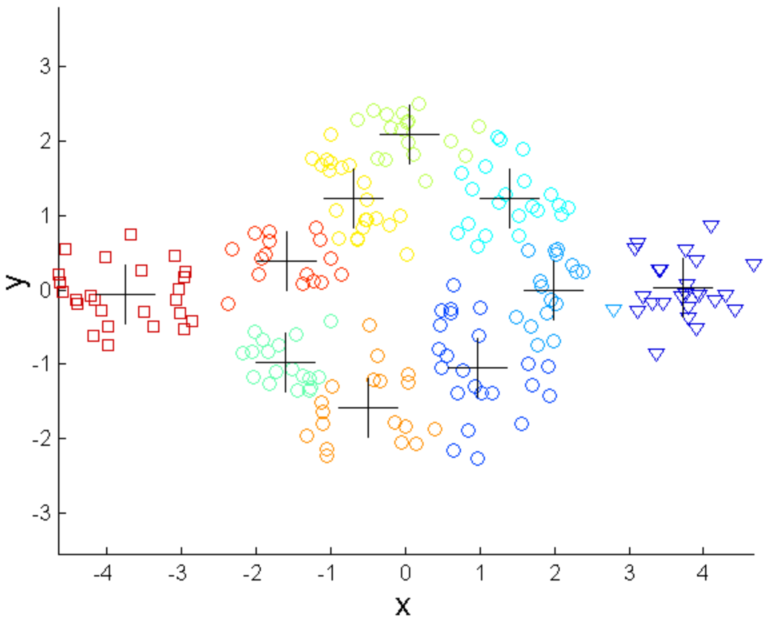
Original Points



K-means (2 Clusters)

Overcoming K-means Limitations





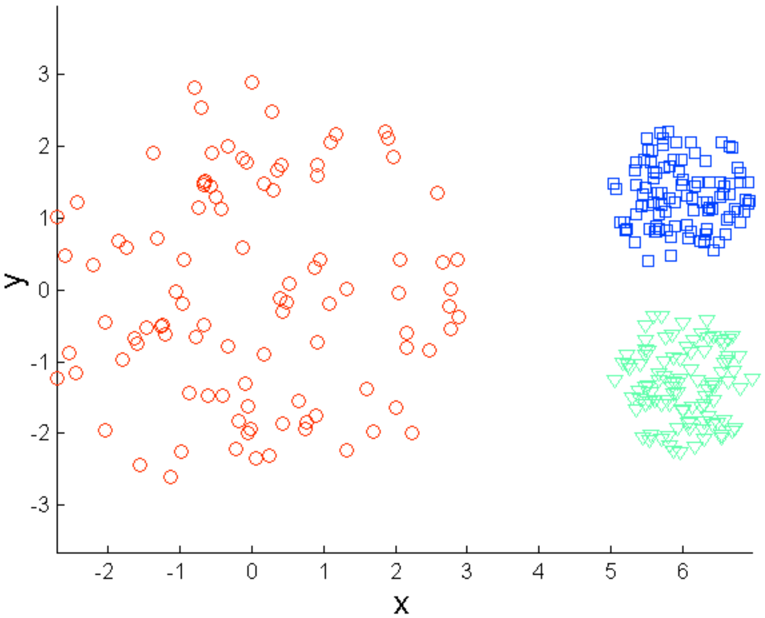
Original Points

K-means Clusters

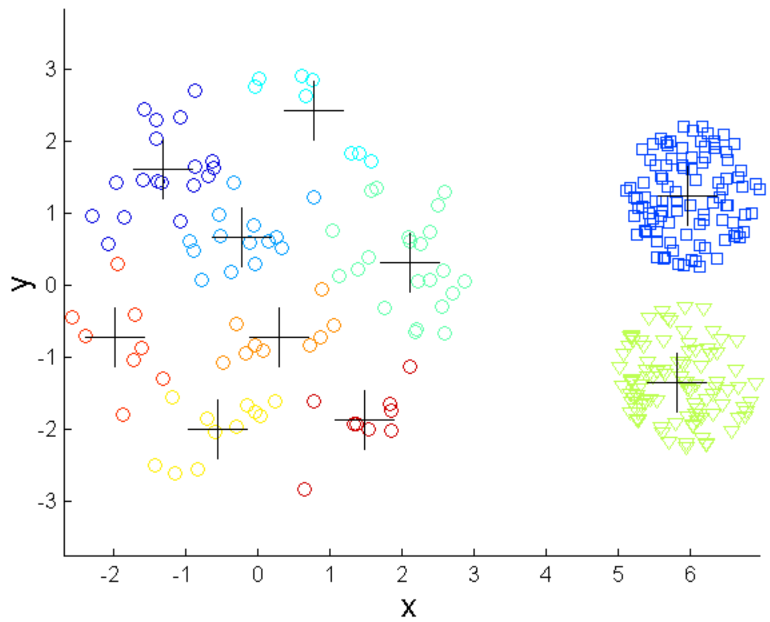
One solution is to use many clusters.

Find parts of clusters, but need to put together.

Overcoming K-means Limitations

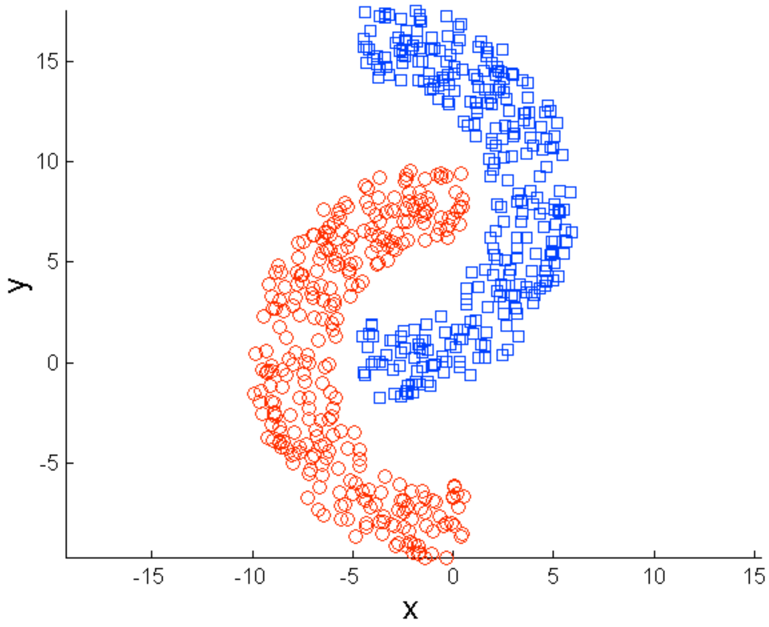


Original Points

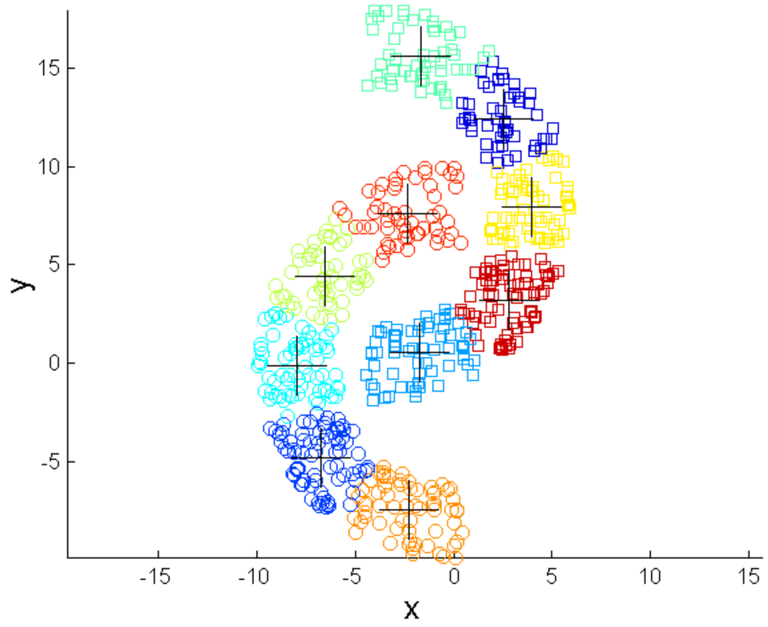


K-means Clusters

Overcoming K-means Limitations



Original Points



K-means Clusters

Variations

- K-medoids: Similar problem definition as in K-means, but the centroid of the cluster is defined to be one of the points in the cluster (the medoid).

- K-centers: Similar problem definition as in K-means, but the goal now is to minimize the maximum diameter of the clusters (diameter of a cluster is maximum distance between any two points in the cluster).