THE UNIVERSITY OF
MELBOURNE

COMP90049 Knowledge Technologies

Clustering
(Lecture Set 9)**2013**

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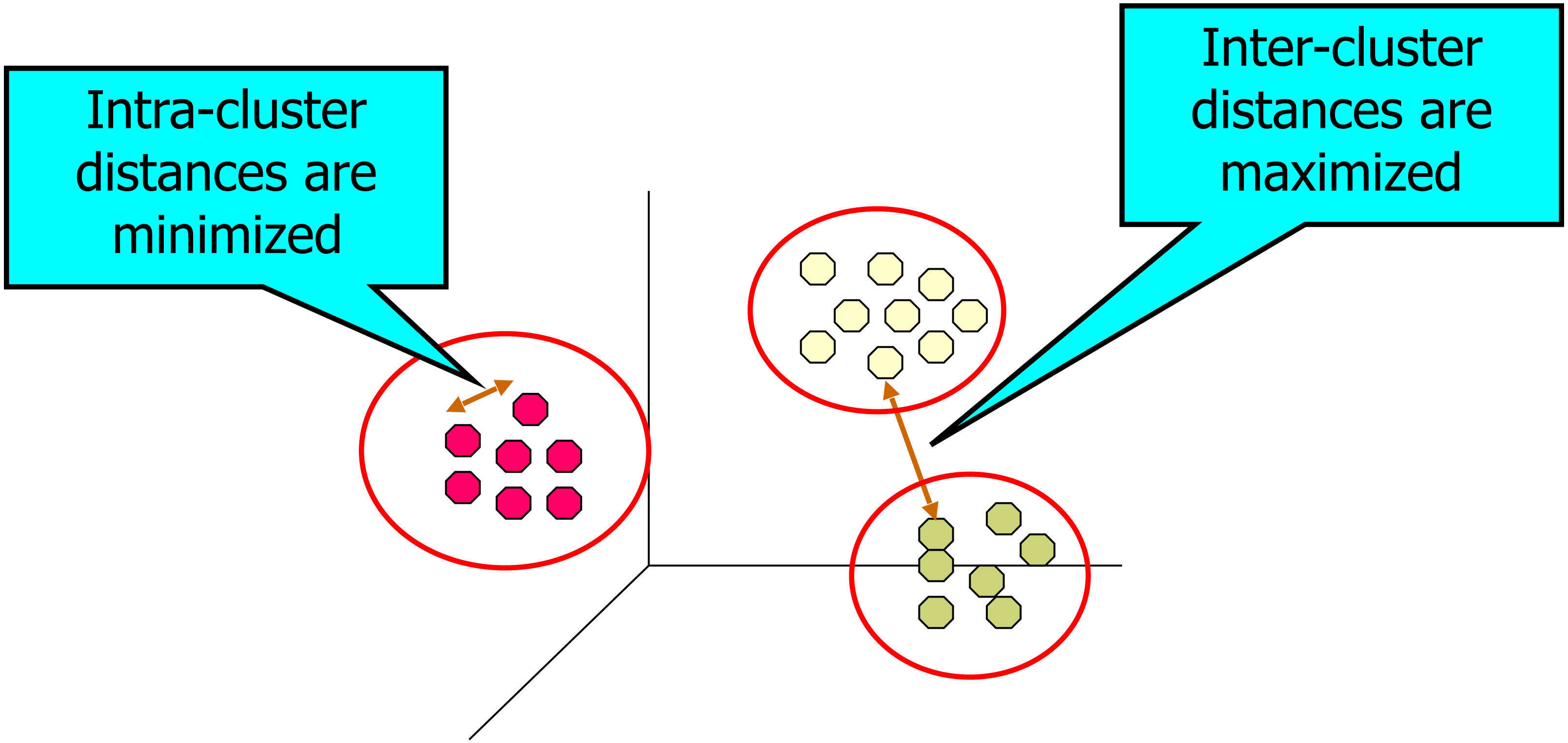
Some of slides are derived from Prof Vipin Kumar and modified, http://www-users.cs.umn.edu/~kumar/

What is Cluster Analysis?

Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups. Of course we need define what we mean by "similar"!



Intra-cluster distances are minimized

Inter-cluster distances are maximized

Applications of Cluster Analysis

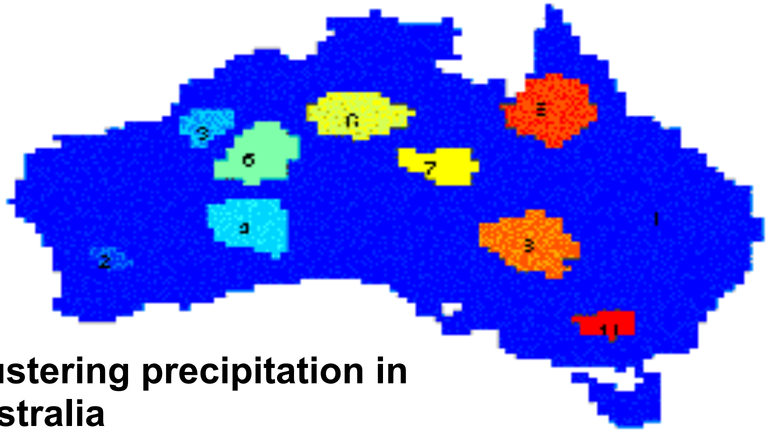
Understanding

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

Summarization

- Reduce the size of large data sets

	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



Clustering precipitation in Australia

What is not Cluster Analysis

Supervised classification

- Have class label information

Simple segmentation

- Dividing students into different registration groups alphabetically, by last name

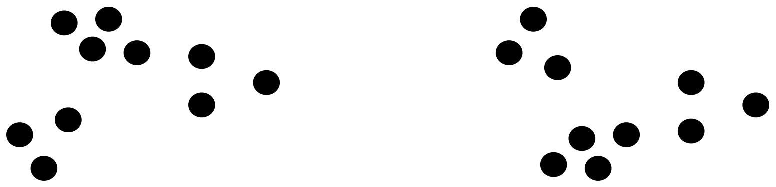
Results of a query

- Groupings are a result of an external specification

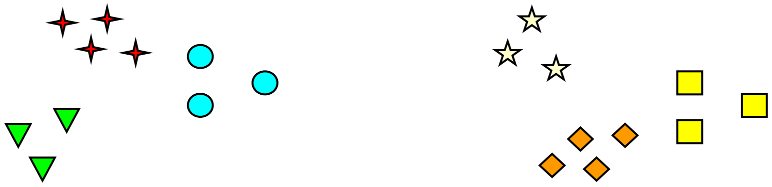
Graph partitioning

- Some mutual relevance and synergy, but areas are not identical

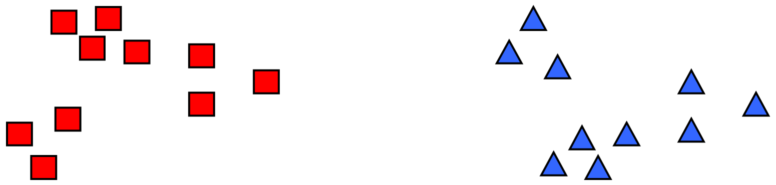
Notion of a Cluster can be Ambiguous



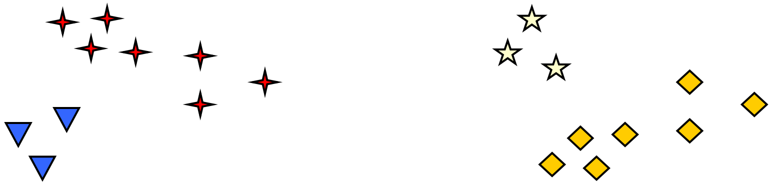
How many clusters?



Six Clusters



Two Clusters



Four Clusters

Types of Clustering

A clustering is a set of clusters

Important distinction between hierarchical and partitional sets of clusters

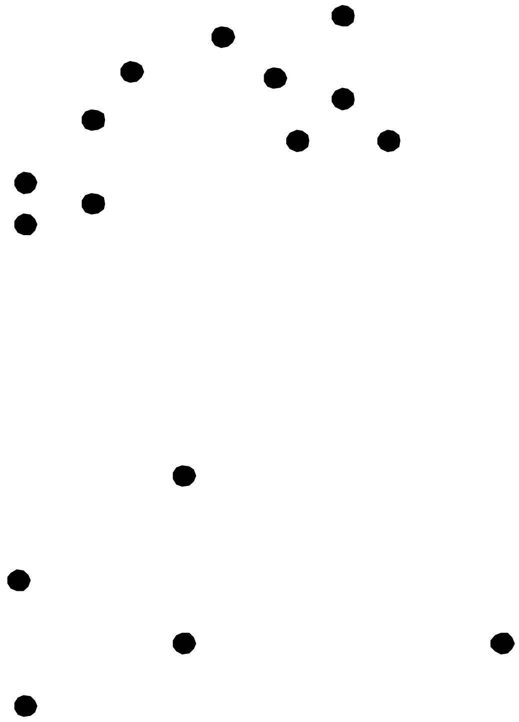
Partitional Clustering

- A division data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset

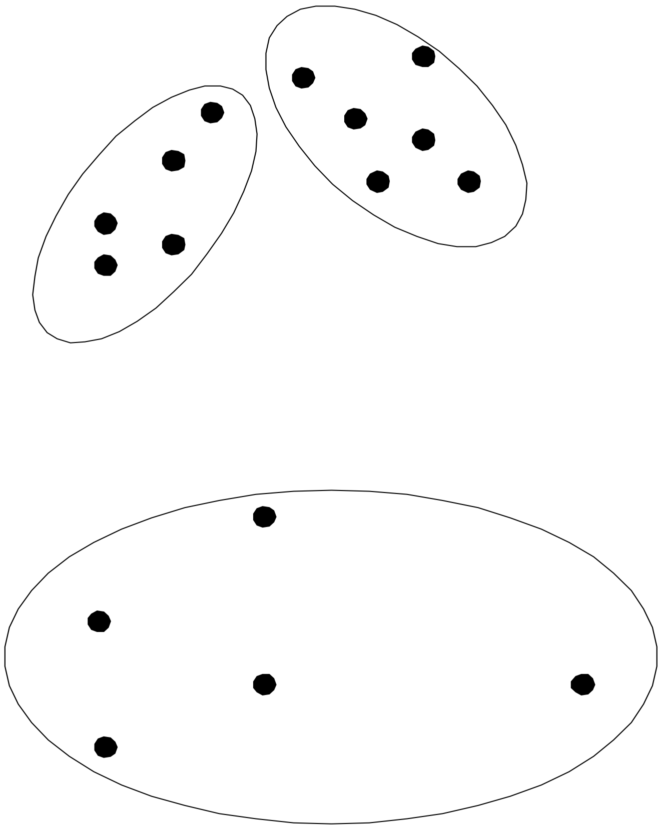
Hierarchical clustering

- A set of nested clusters organized as a hierarchical tree

Partitional Clustering

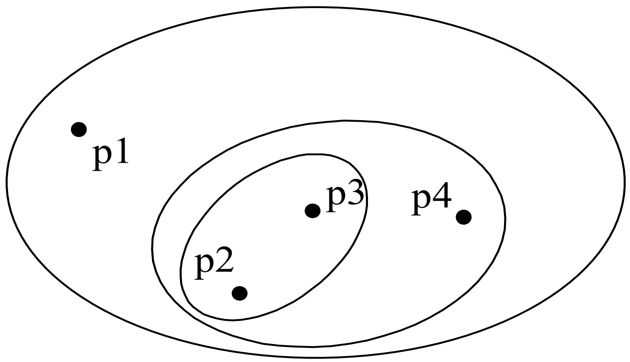


Original Points

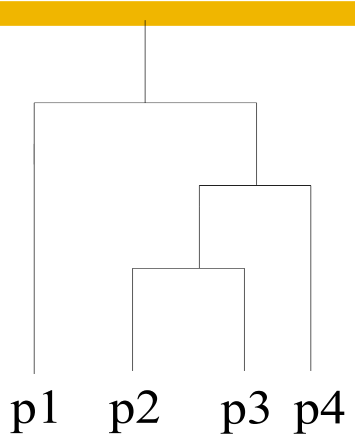


A Partitional Clustering

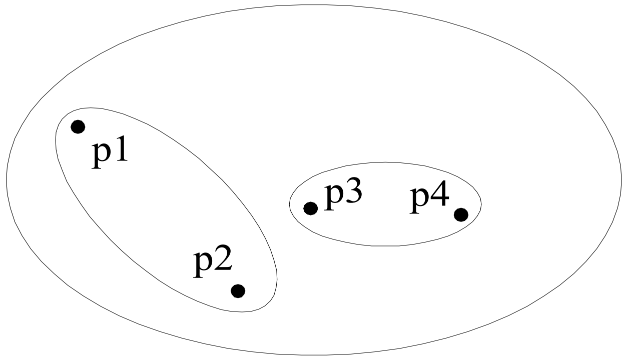
Hierarchical Clustering



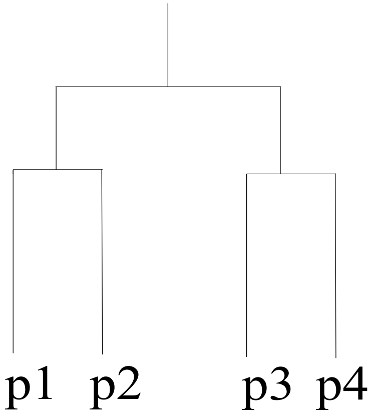
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering



Non-traditional Dendrogram

Other Distinctions Between Sets of Clusters

Exclusive versus non-exclusive

- In non-exclusive clusterings, points may belong to multiple clusters.
- Can represent multiple classes or ‘border’ points

Fuzzy versus non-fuzzy

- In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1
- Weights must sum to 1
- Probabilistic clustering has similar characteristics

Partial versus complete

- In some cases, we only want to cluster some of the data

Heterogeneous versus homogeneous

- Cluster of widely different sizes, shapes, and densities

Types of Clusters

Well-separated clusters

Center-based clusters

Contiguous clusters

Density-based clusters

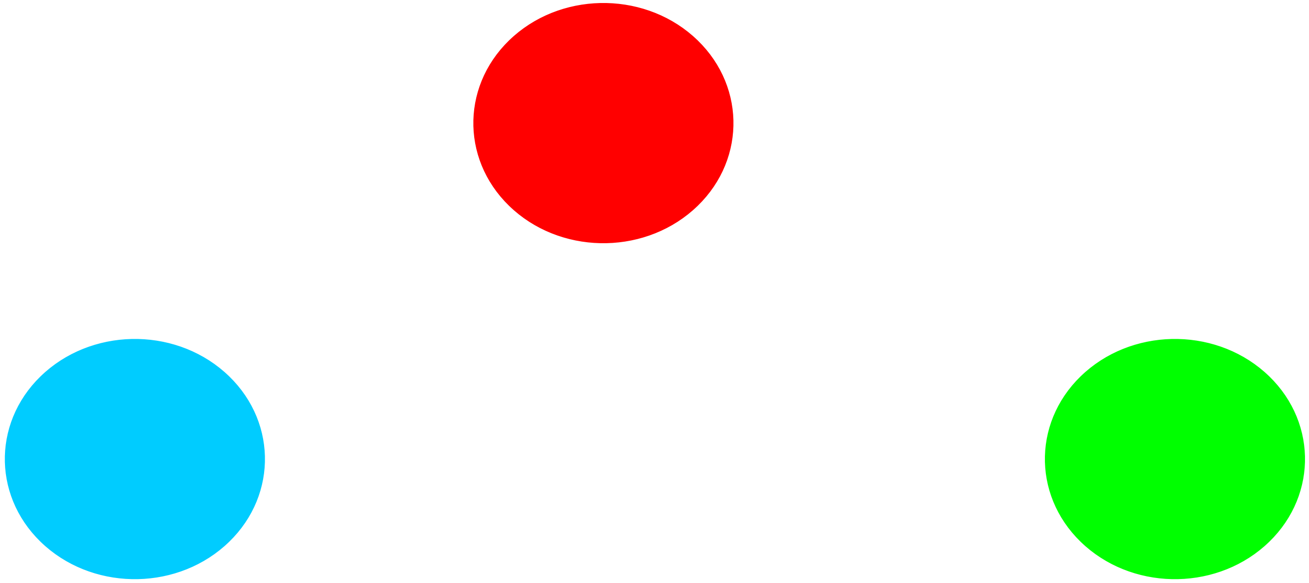
Property or Conceptual

Described by an Objective Function

Types of Clusters: Well-Separated (easiest clustering)

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.

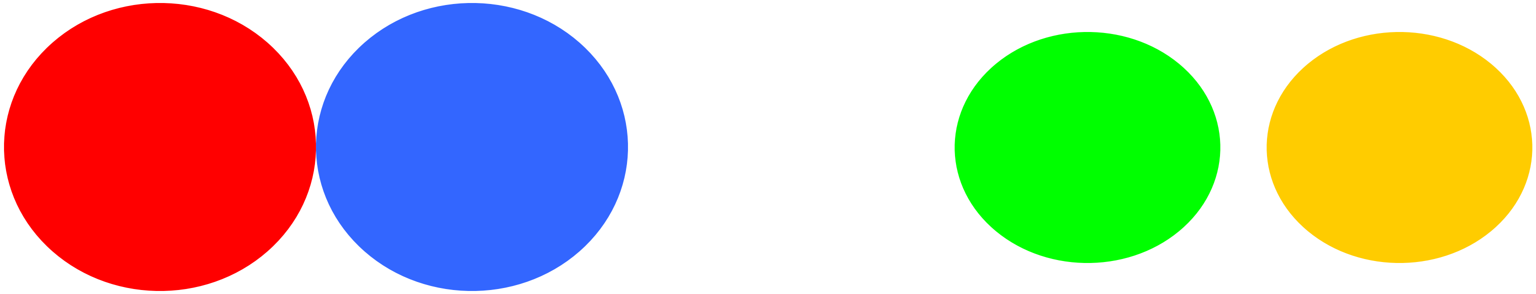


3 well-separated clusters

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 average of all the points in the cluster, or a medoid, the most "representative" point of a cluster

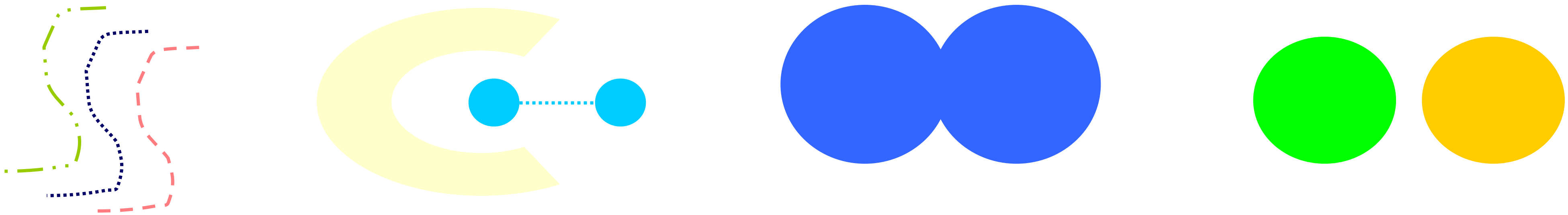


4 center-based clusters

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.

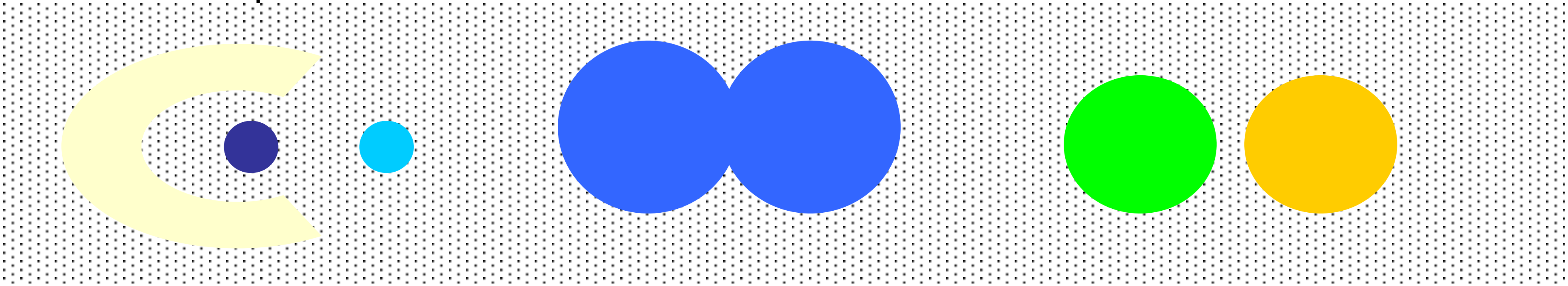


8 contiguous clusters

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.

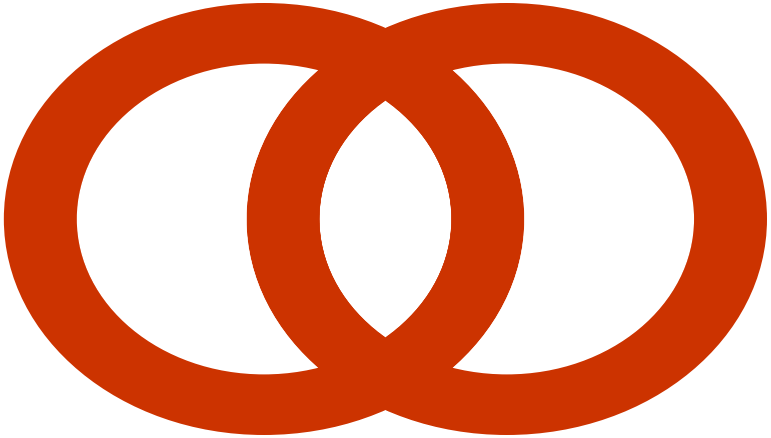


6 density-based clusters

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

Clusters Defined by an Objective Function

- 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.

  Parameters for the model are determined from the data.

  Mixture models assume that the data is a ‘mixture' of a number of statistical distributions.

Types of Clusters: Objective Function …

Map the clustering problem to a different domain and solve a related problem in that domain

- Proximity matrix defines a weighted graph, where the nodes are the points being clustered, and the weighted edges represent the proximities between points
- Clustering is equivalent to breaking the graph into connected components, one for each cluster.
- Want to minimize the edge weight between clusters and maximize the edge weight within clusters

Characteristics of the Input Data Are Important

Type of proximity or density measure

- This is a derived measure, but central to clustering

Sparseness

- Dictates type of similarity
- Adds to efficiency

Attribute type

- Dictates type of similarity

Type of Data

- Dictates type of similarity
- Other characteristics, e.g., autocorrelation

Dimensionality

Noise and Outliers

Type of Distribution

Clustering Algorithms

K-means and its variants

Hierarchical clustering

Density-based clustering

K-means Clustering

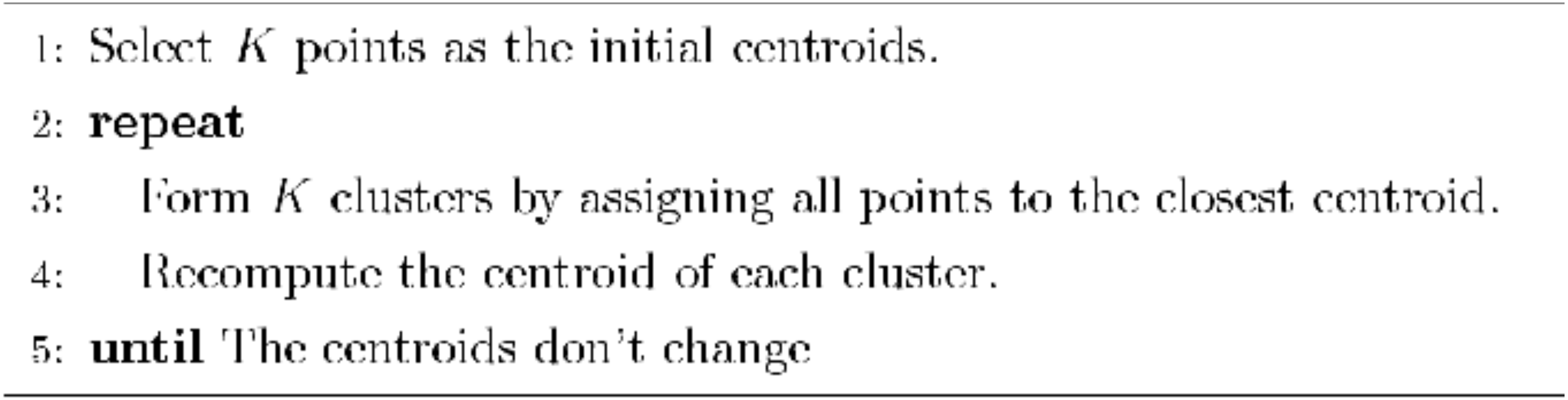
Partitional clustering approach

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 basic algorithm is very simple



```
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 Clustering – Details

Initial centroids are often chosen randomly.

- Clusters produced vary from one run to another.

The centroid is (typically) the mean of the points in the cluster.

'Closeness' is measured by Euclidean distance, cosine similarity, correlation, etc.

K-means will converge for common similarity measures mentioned above.

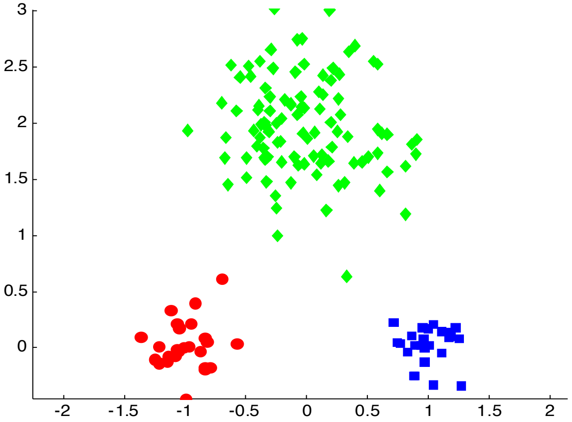
Most of the convergence happens in the first few iterations.

- Often the stopping condition is changed to 'Until relatively few points change clusters' (this way the stopping criterion will not depend on the type of similarity or dimensionality)

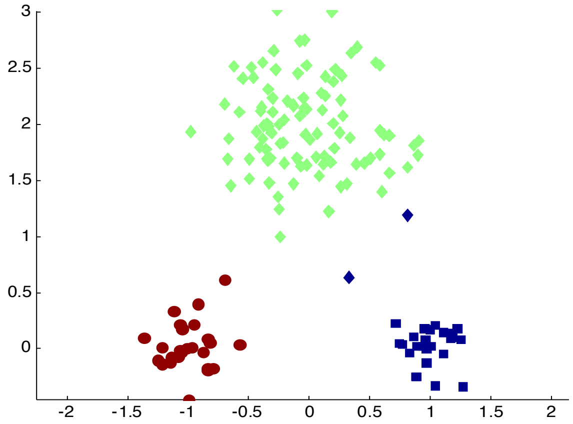
Complexity is O(n * K * I * d)

- n = number of points, K = number of clusters,
  I = number of iterations, d = number of attributes
- Unfortunately we cannot a priory know the value of I!

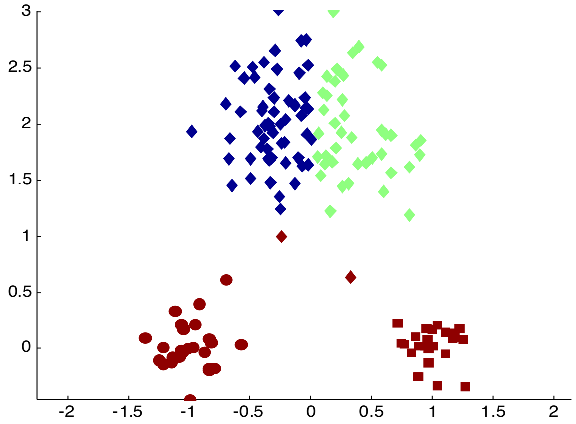
Two different K-means Clusterings



Original Points

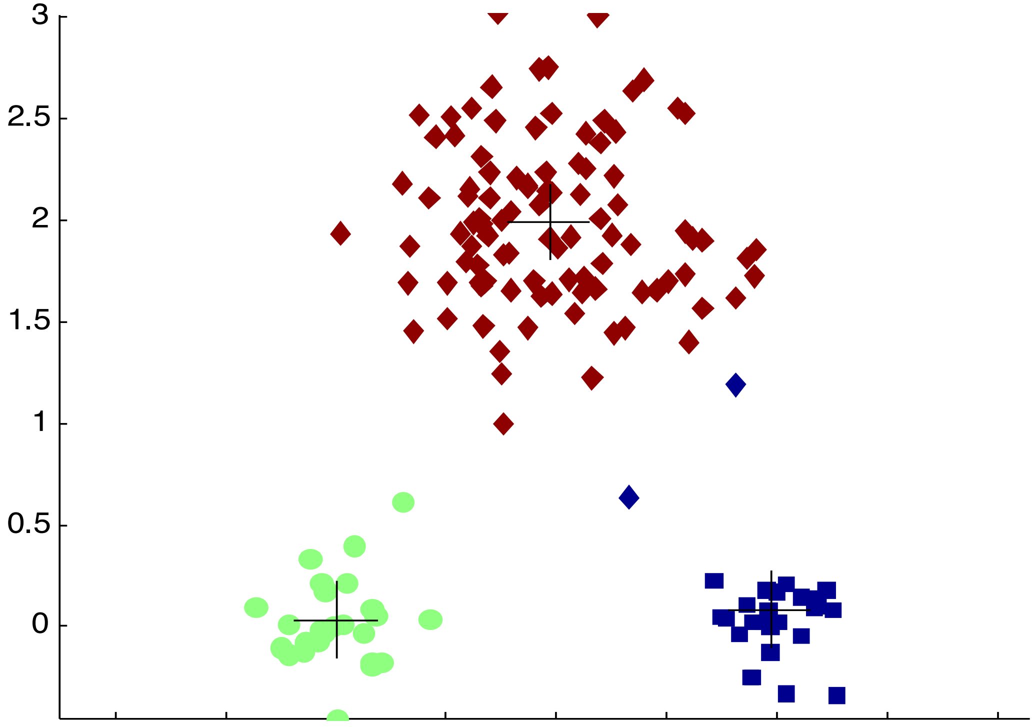


Optimal Clustering

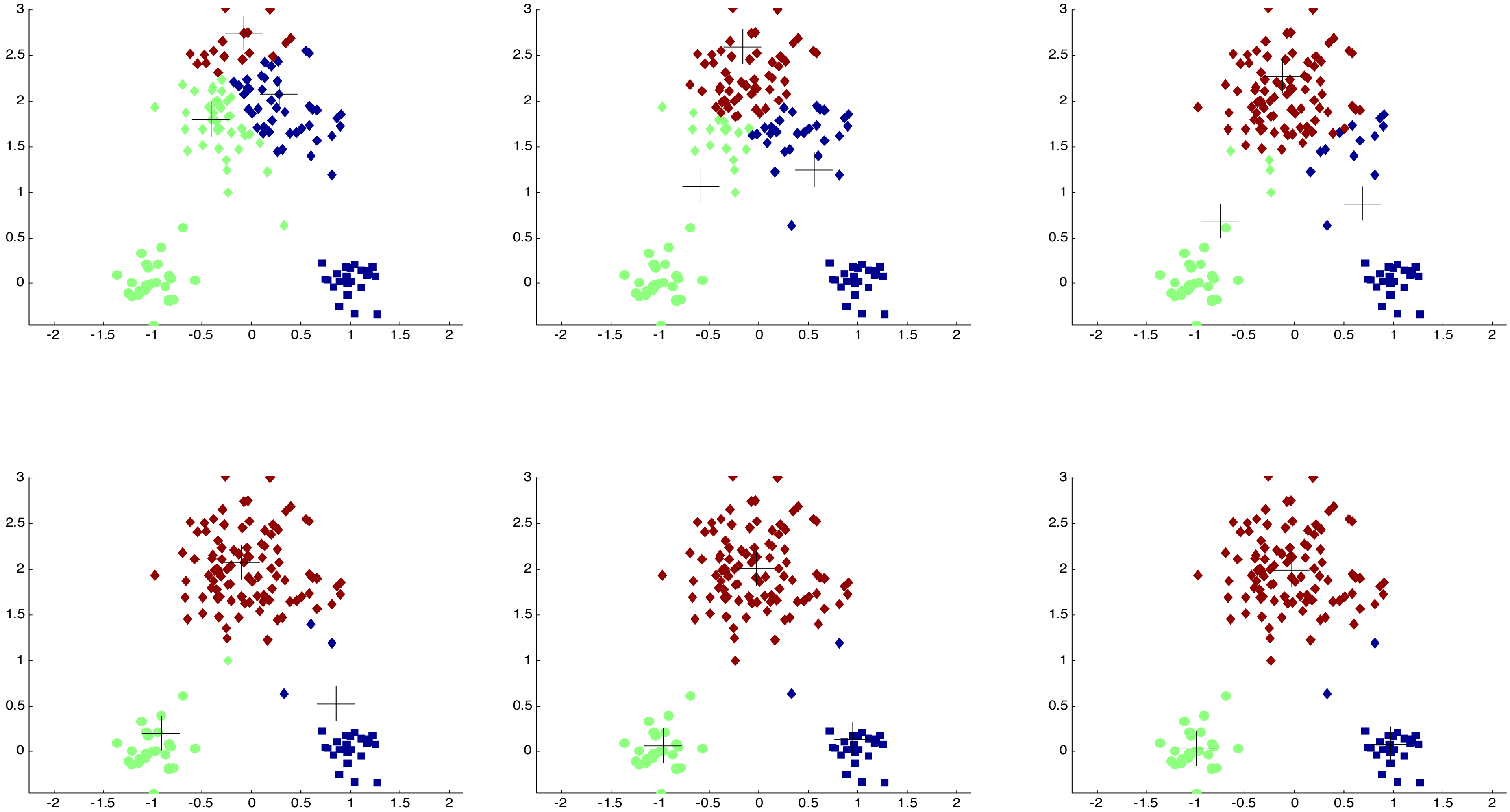


Sub-optimal Clustering

Importance of Choosing Initial Centroids



Importance of Choosing Initial Centroids



Evaluating K-means Clusters

Most common measure is Sum of Squared Error (SSE)

- For each point, the error is the distance to the nearest cluster
- To get SSE, we square these errors and sum them.

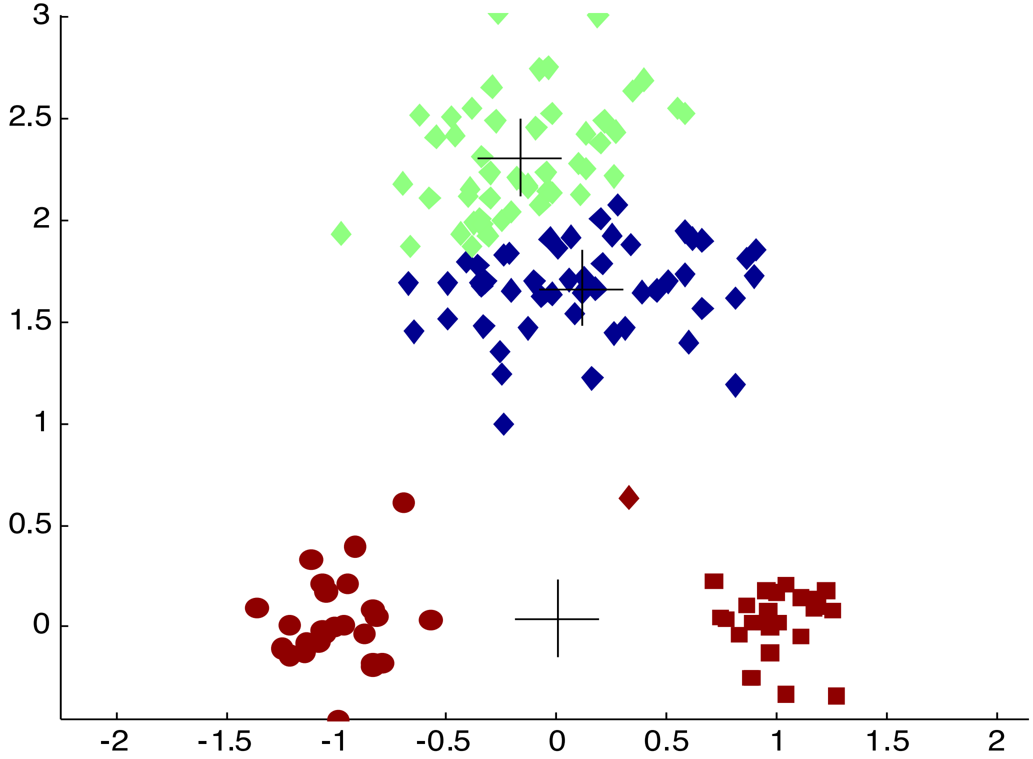
$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x)$$

- *x* is a data point in cluster C_i and m_i is the representative point for cluster C_i

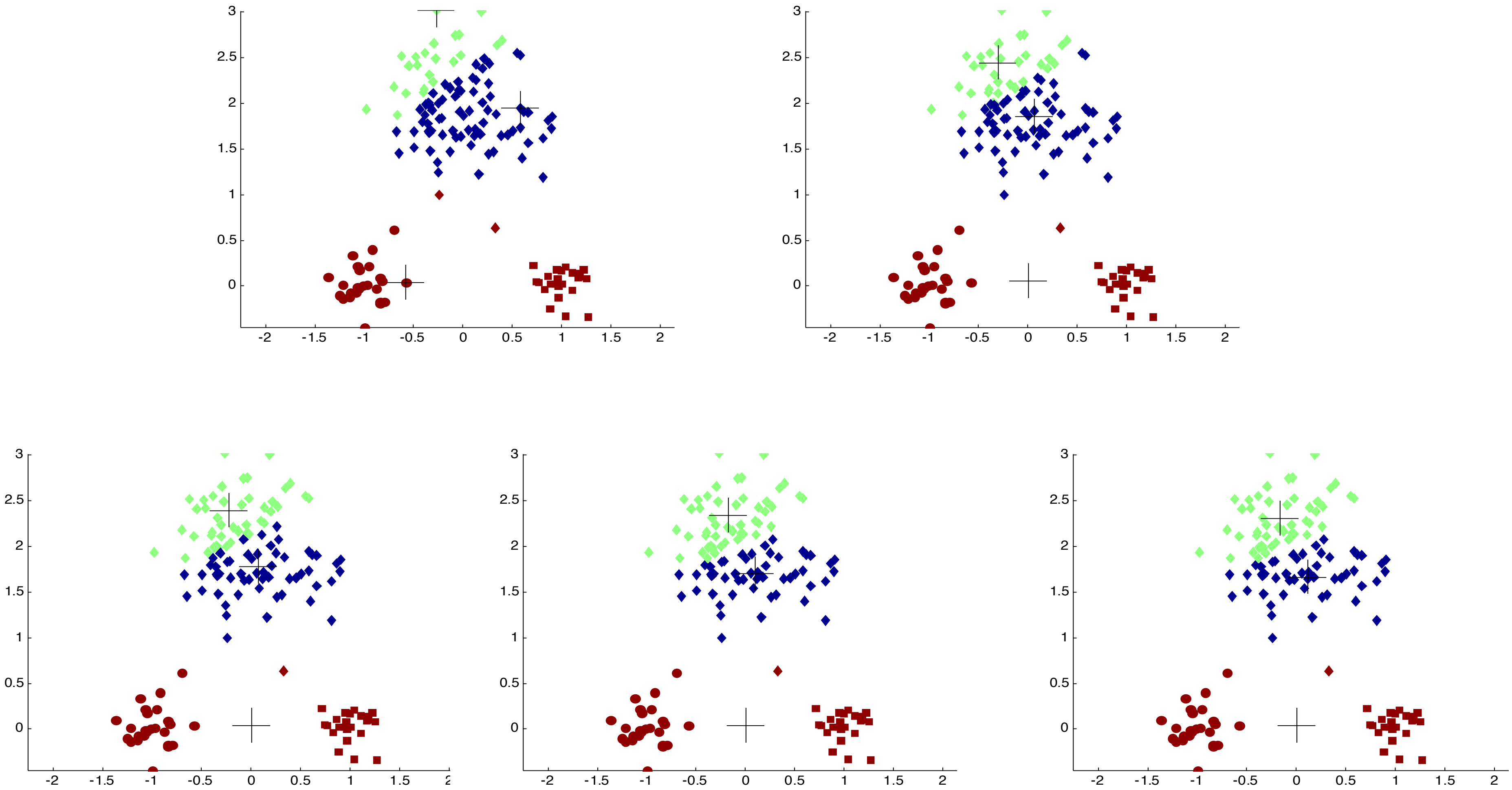
  can show that m_i corresponds to the center (mean) of the cluster
- Given two clusters, we can choose the one with the smallest error
- One easy way to reduce SSE is to increase K, the number of clusters

  A good clustering with smaller K can have a lower SSE than a poor clustering with higher K

Importance of Choosing Initial Centroids …



Importance of Choosing Initial Centroids …



Problems with Selecting Initial Points

If there are K ‘real’ clusters then the chance of selecting one centroid from each cluster is small.

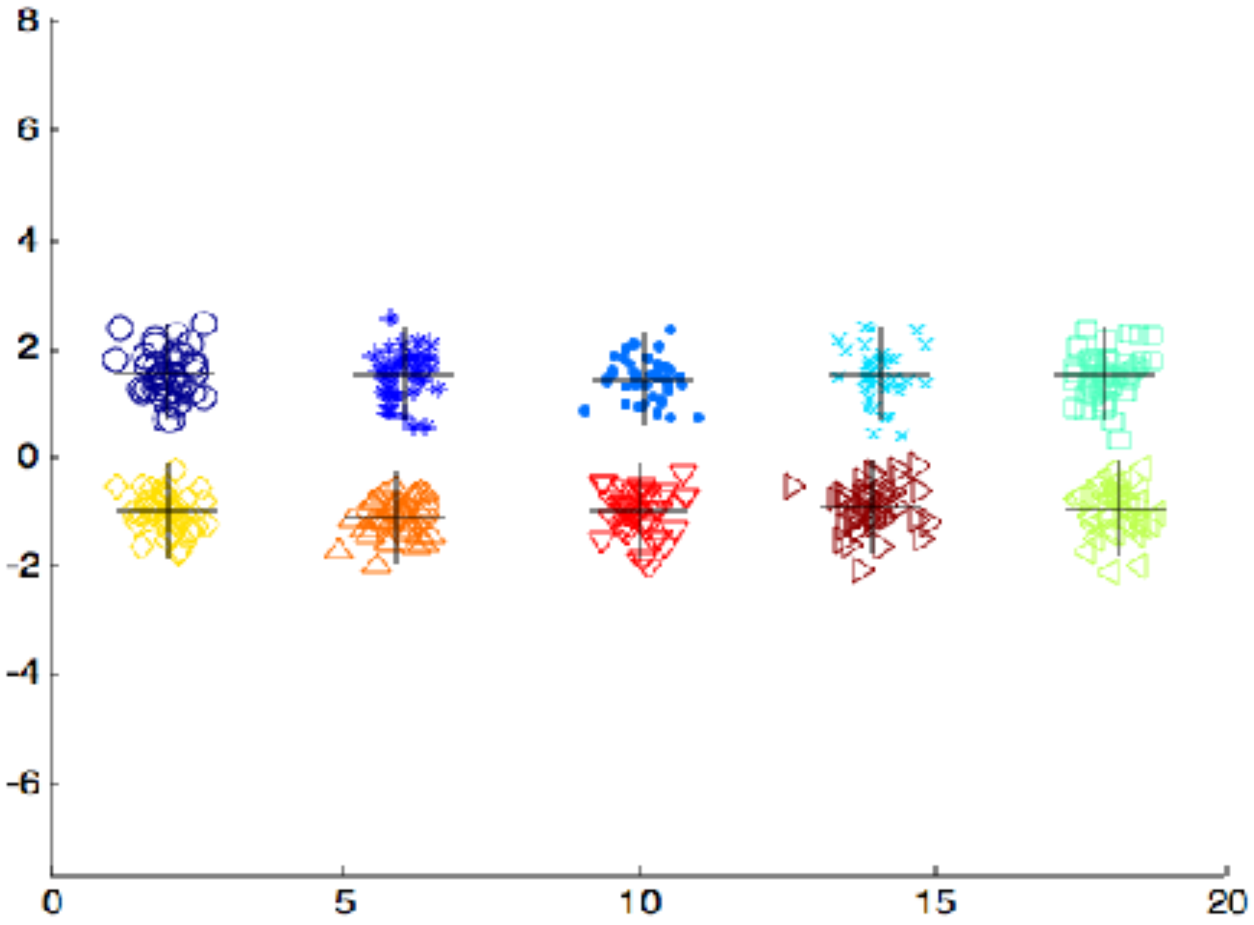
- Chance is relatively small when K is large
- If clusters are the same size, n, then

$$P = \frac{\#\text{ of ways to select one centroid from each cluster}}{\#\text{ of ways to select K centroids}} = \frac{\binom{n}{1}^K}{\binom{nK}{K}} \cong \frac{n^K}{\frac{(nK)^K}{K!}}$$

$$= \frac{K!}{K^K}$$

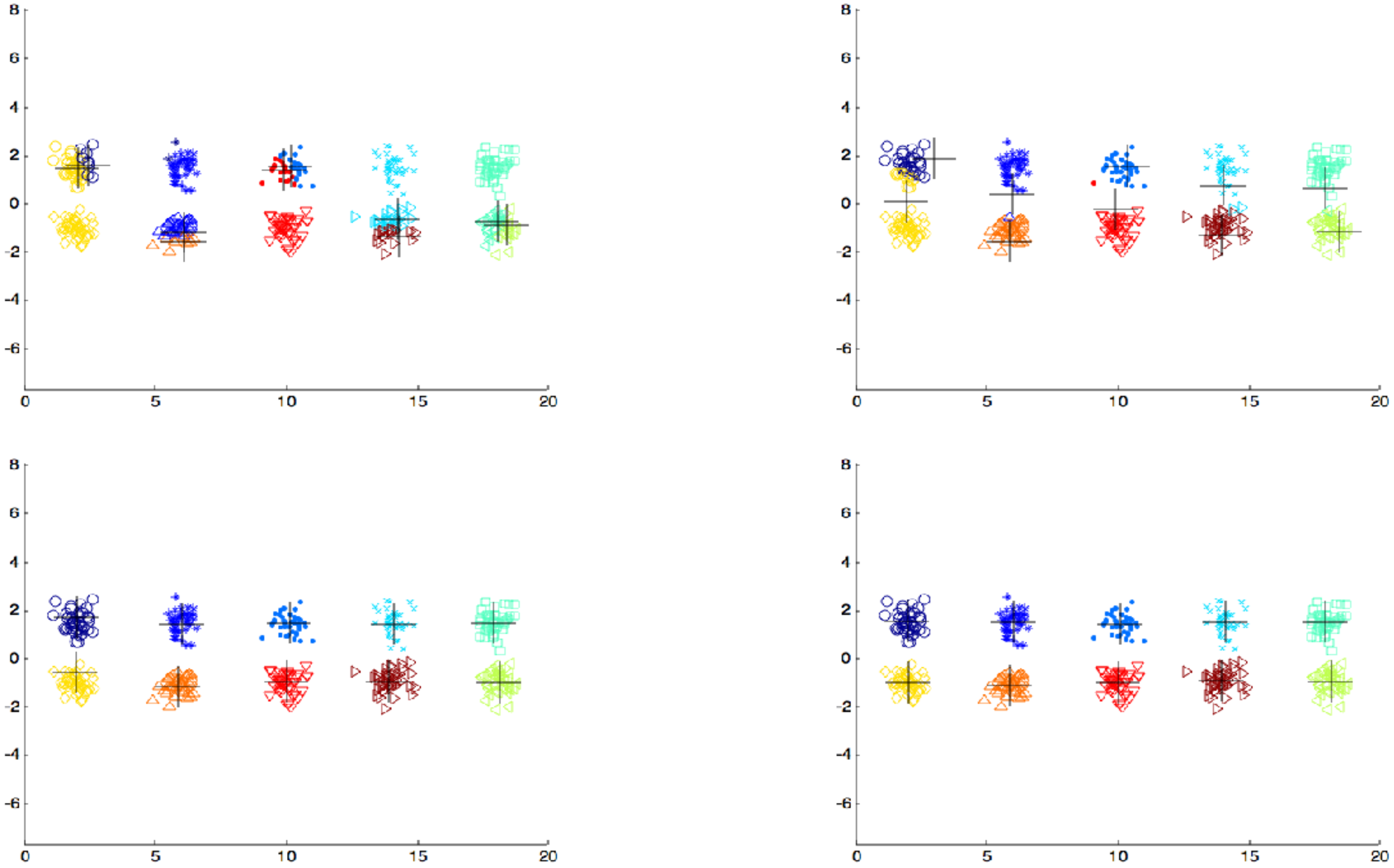
- For example, if K = 10, then probability = $10!/10^{10}$ = 0.00036
- Sometimes the initial centroids will readjust themselves in ‘right’ way, and sometimes they don’t
- Consider an example of five pairs of clusters

10 Clusters Example



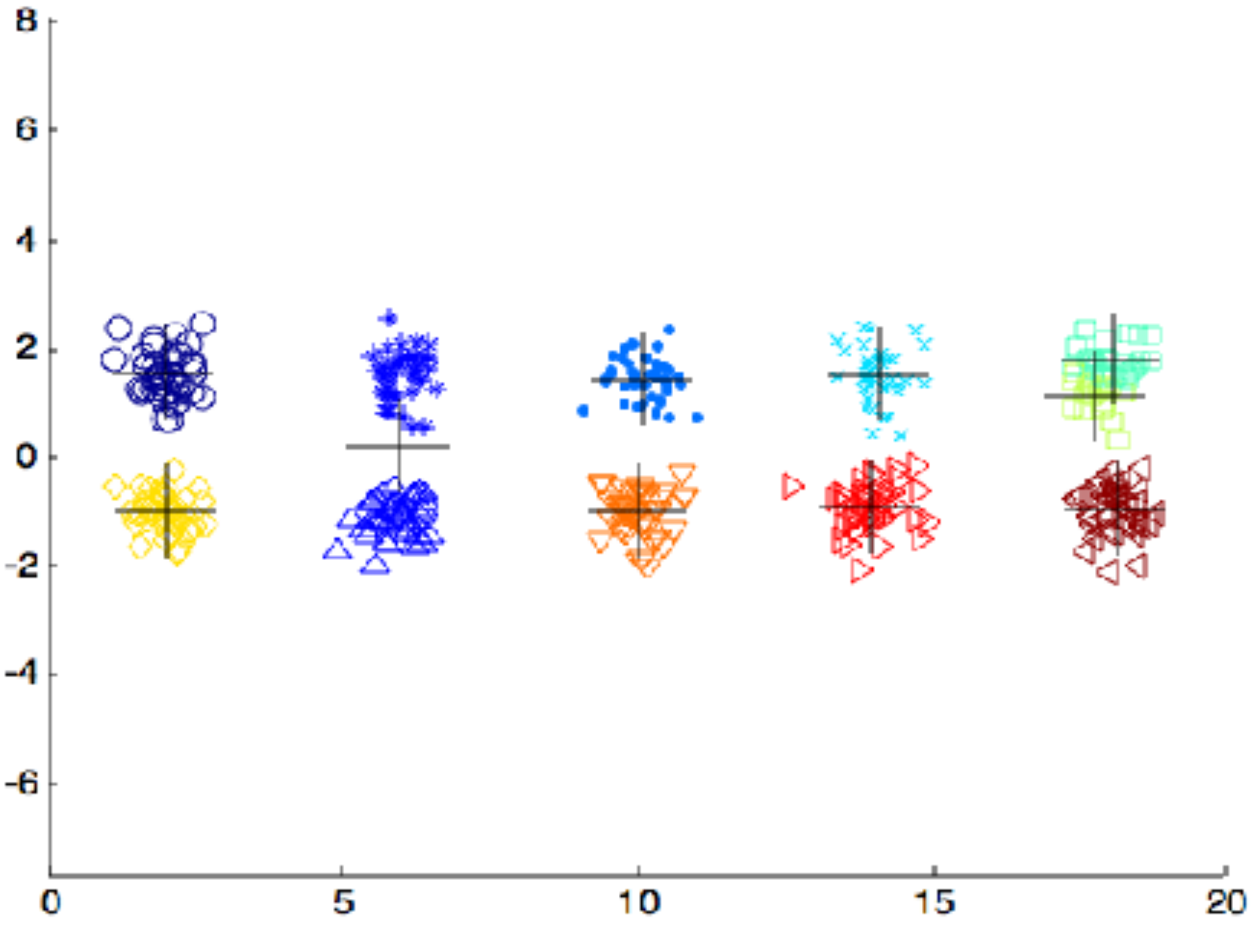
Starting with two initial centroids in one cluster of each pair of clusters

10 Clusters Example



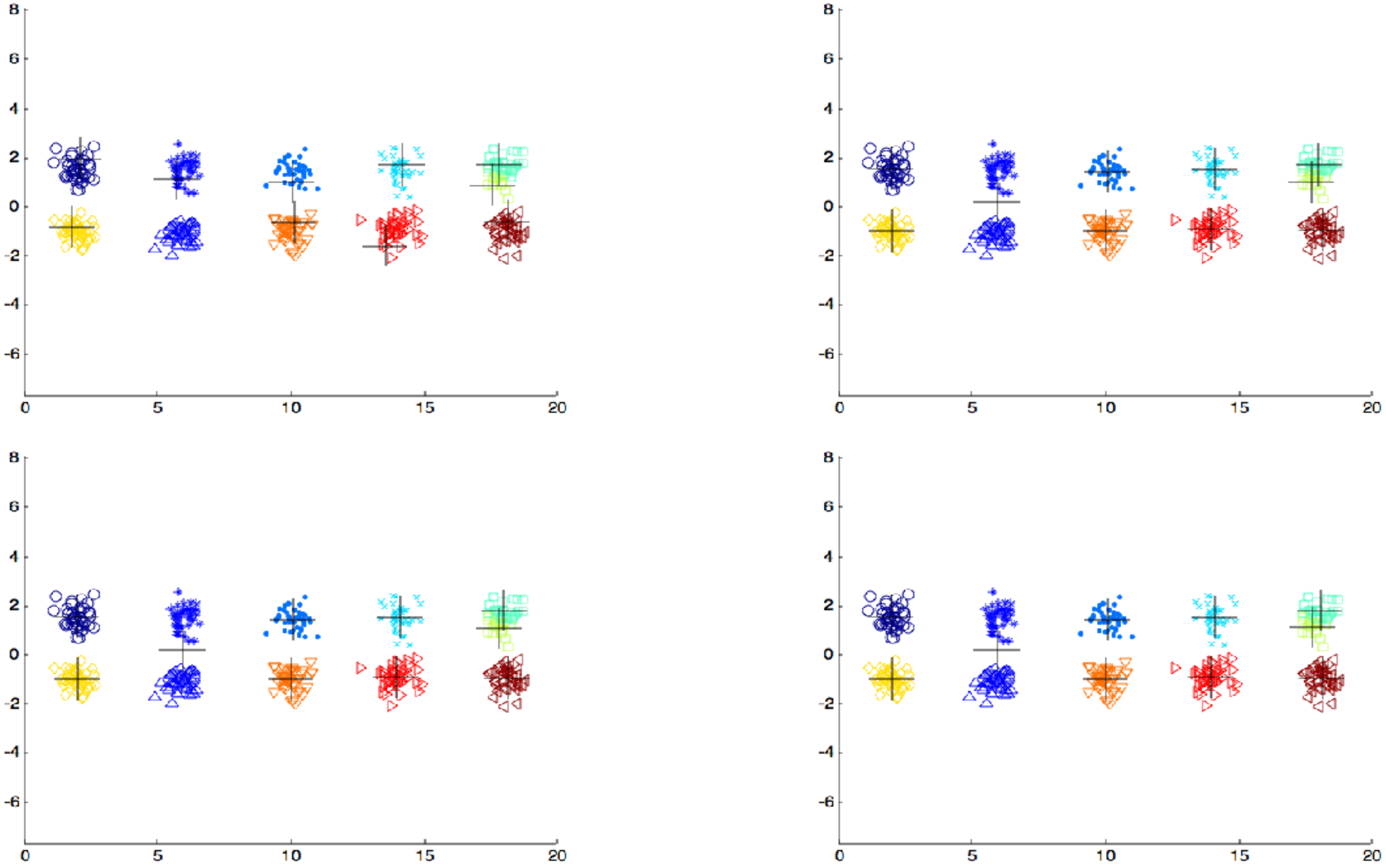
Starting with two initial centroids in one cluster of each pair of clusters

10 Clusters



Starting with some pairs of clusters having three initial centroids, while other have only one.

10 Clusters Example



Starting with some pairs of clusters having three initial centroids, while other have only one.

Solutions to Initial Centroids Problem

Multiple runs

- Helps, but probability is not on your side

Sample and use hierarchical clustering to determine initial centroids

Select more than k initial centroids and then select among these initial centroids

- Select most widely separated

Postprocessing

Bisecting K-means

- Not as susceptible to initialization issues

Handling Empty Clusters

Basic K-means algorithm can yield empty clusters

Several strategies

- Choose the point that contributes most to SSE
- Choose a point from the cluster with the highest SSE
- If there are several empty clusters, the above can be repeated several times.

Updating Centers Incrementally

In the basic K-means algorithm, centroids are updated after all points are assigned to a centroid

An alternative is to update the centroids after each assignment (incremental approach)

- Each assignment updates zero or two centroids
- More expensive
- Introduces an order dependency
- Never get an empty cluster
- Can use “weights” to change the impact

Pre-processing and Post-processing

Pre-processing

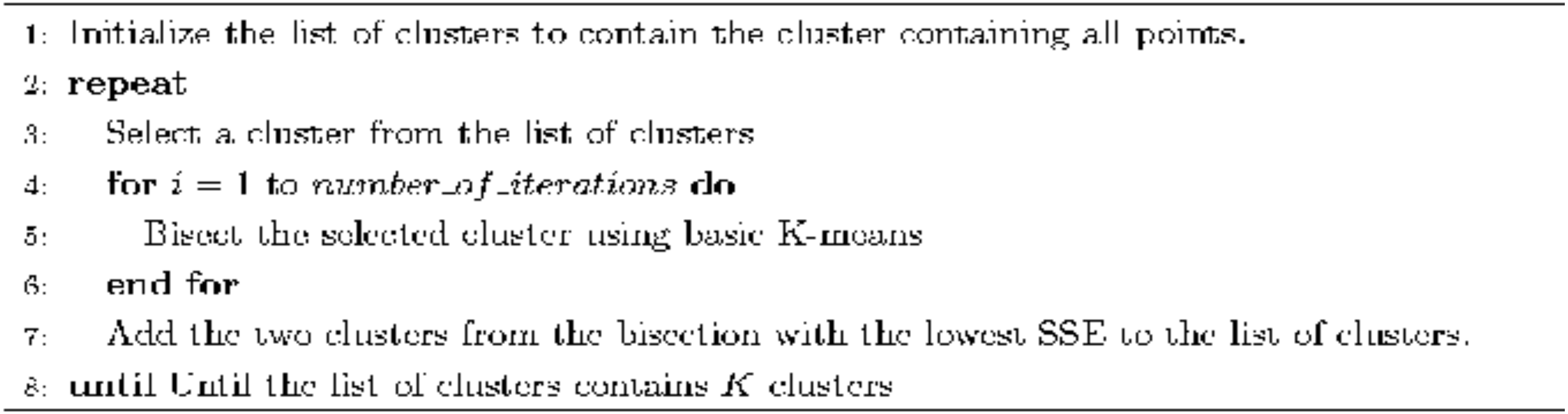
- Normalize the data
- Eliminate outliers

Post-processing

- Eliminate small clusters that may represent outliers
- Split ‘loose’ clusters, i.e., clusters with relatively high SSE
- Merge clusters that are ‘close’ and that have relatively low SSE
- Can use these steps during the clustering process

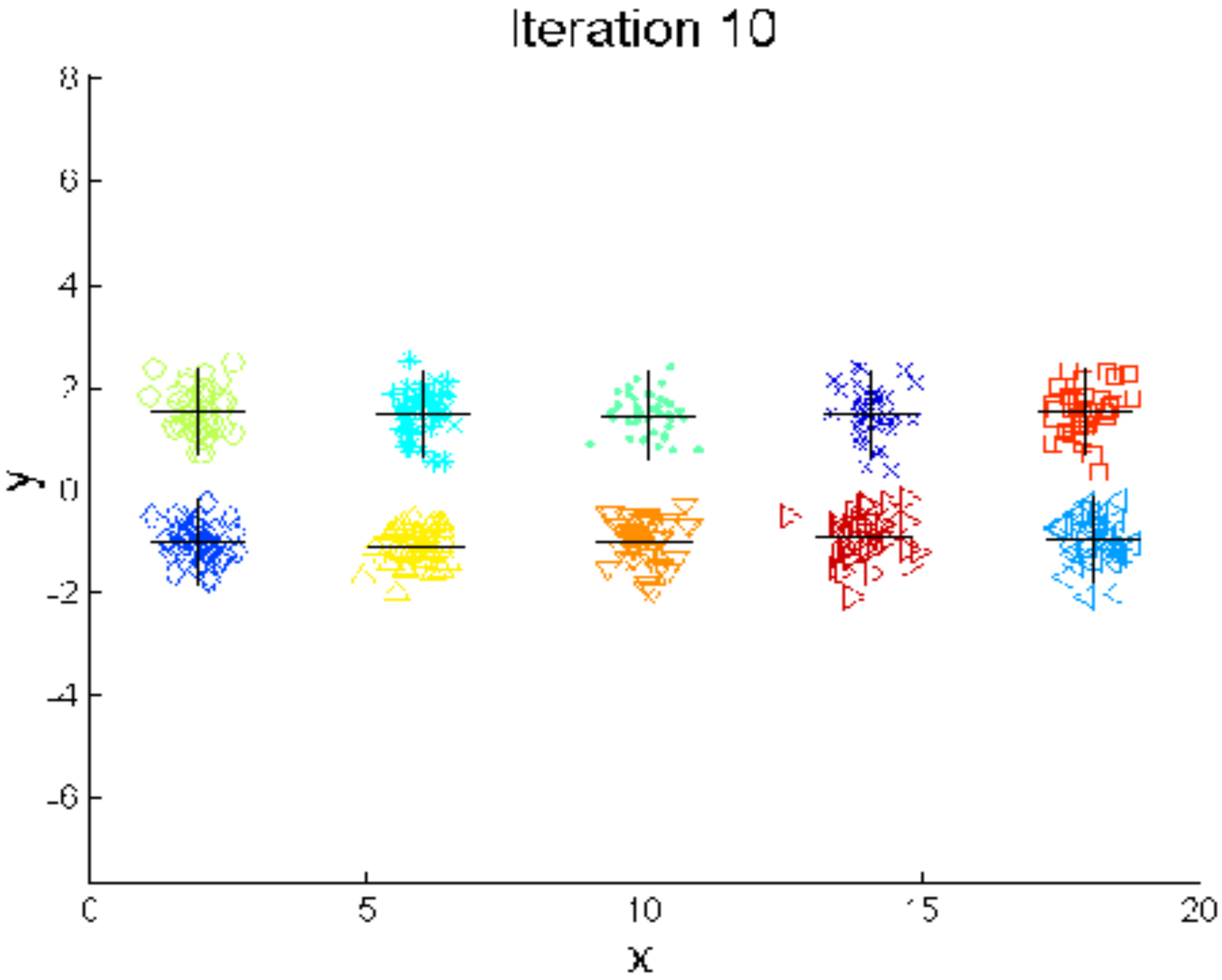
Bisecting K-means algorithm

- Variant of K-means that can produce a partitional or a hierarchical clustering



```
Initialize the list of clusters to contain the cluster containing all points.
repeat
    Select a cluster from the list of clusters
    for $i = 1$ to $number\_of\_iterations$ do
        Bisect the selected cluster using basic K-means
    end for
    Add the two clusters from the bisection with the lowest SSE to the list of clusters.
until Until the list of clusters contains $K$ clusters
```

Bisecting K-means Example



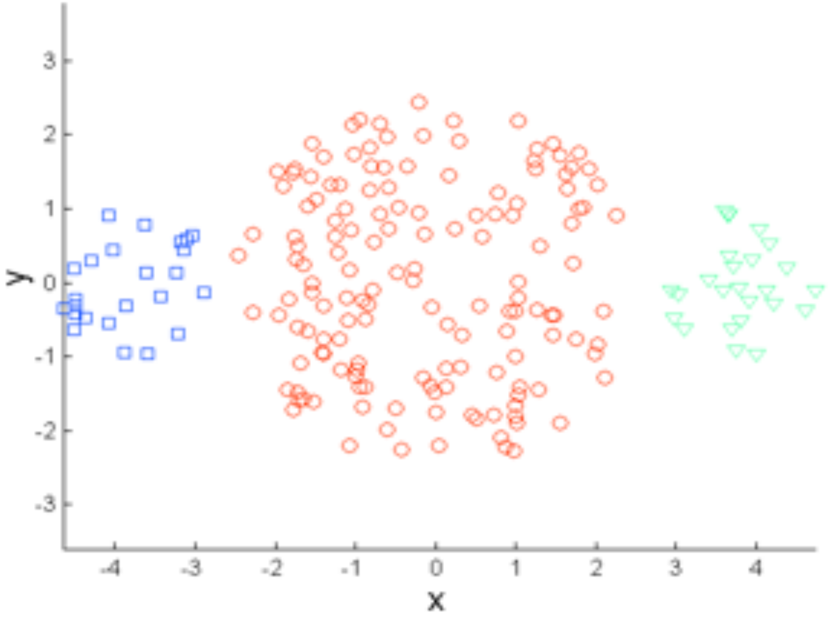
Limitations of K-means

K-means has problems when clusters are of differing

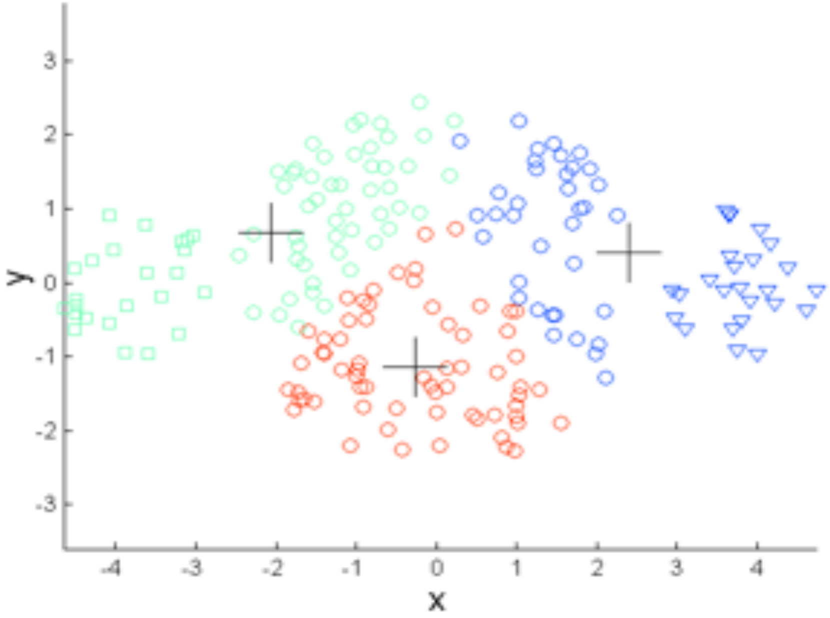
- Sizes
- Densities
- Non-globular shapes

K-means has problems when the data contains outliers.

Limitations of K-means: Differing Sizes

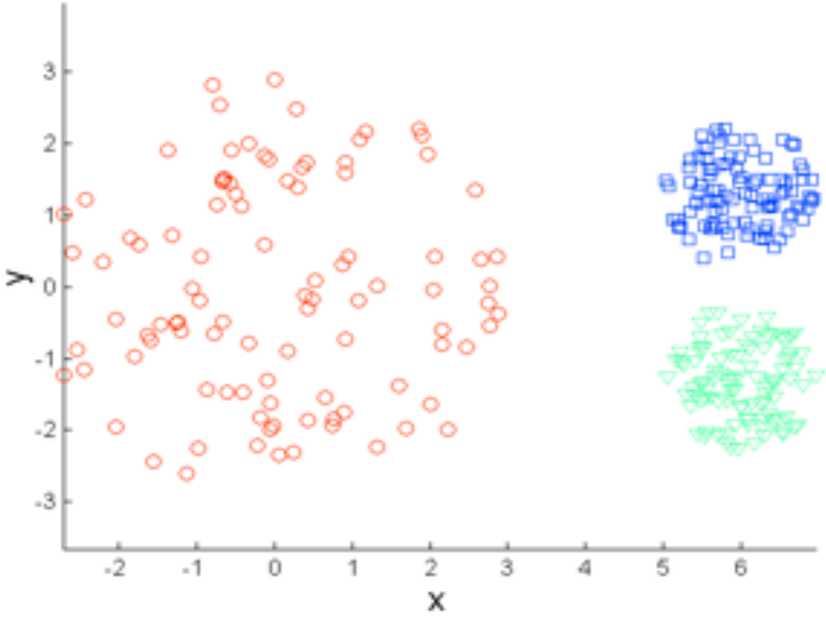


Original Points

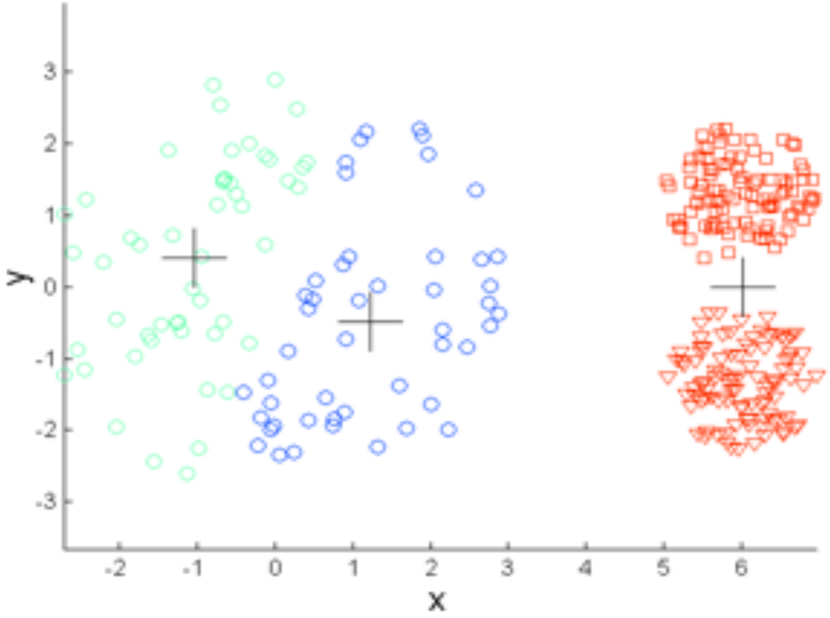


K-means (3 Clusters)

Limitations of K-means: Differing Density

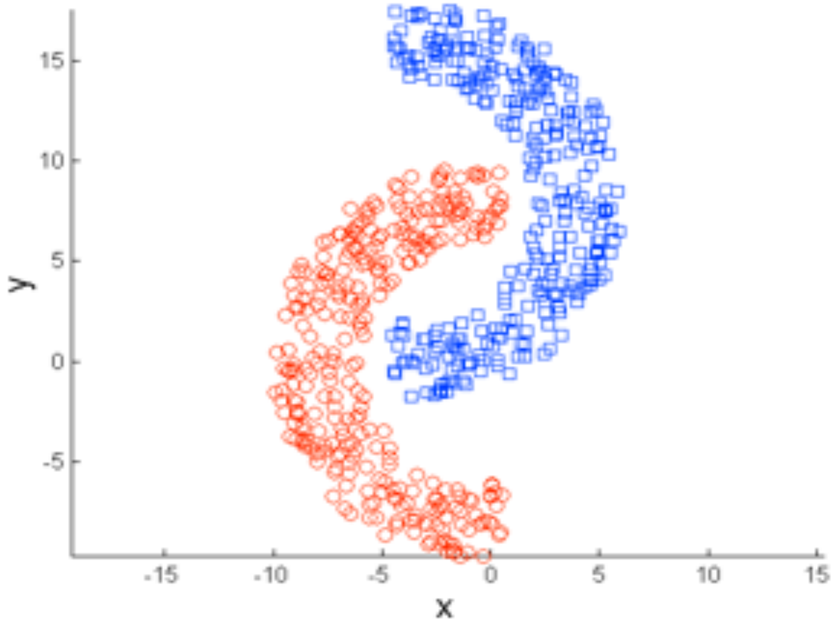


Original Points

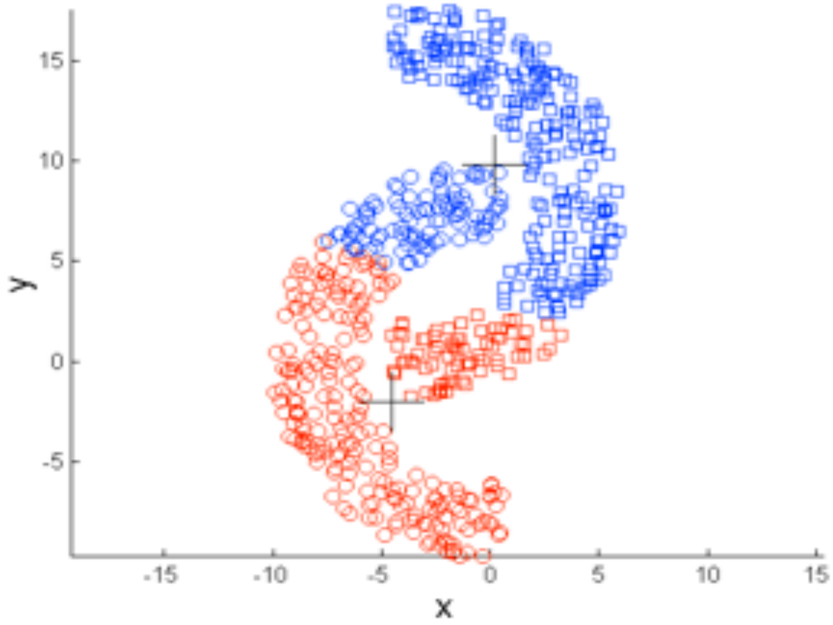


K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes



Original Points



K-means (2 Clusters)

Final Comment on Clustering

Clustering is in the eyes of the beholder

"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**