Introduction to Machine Learning Applications

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Clustering

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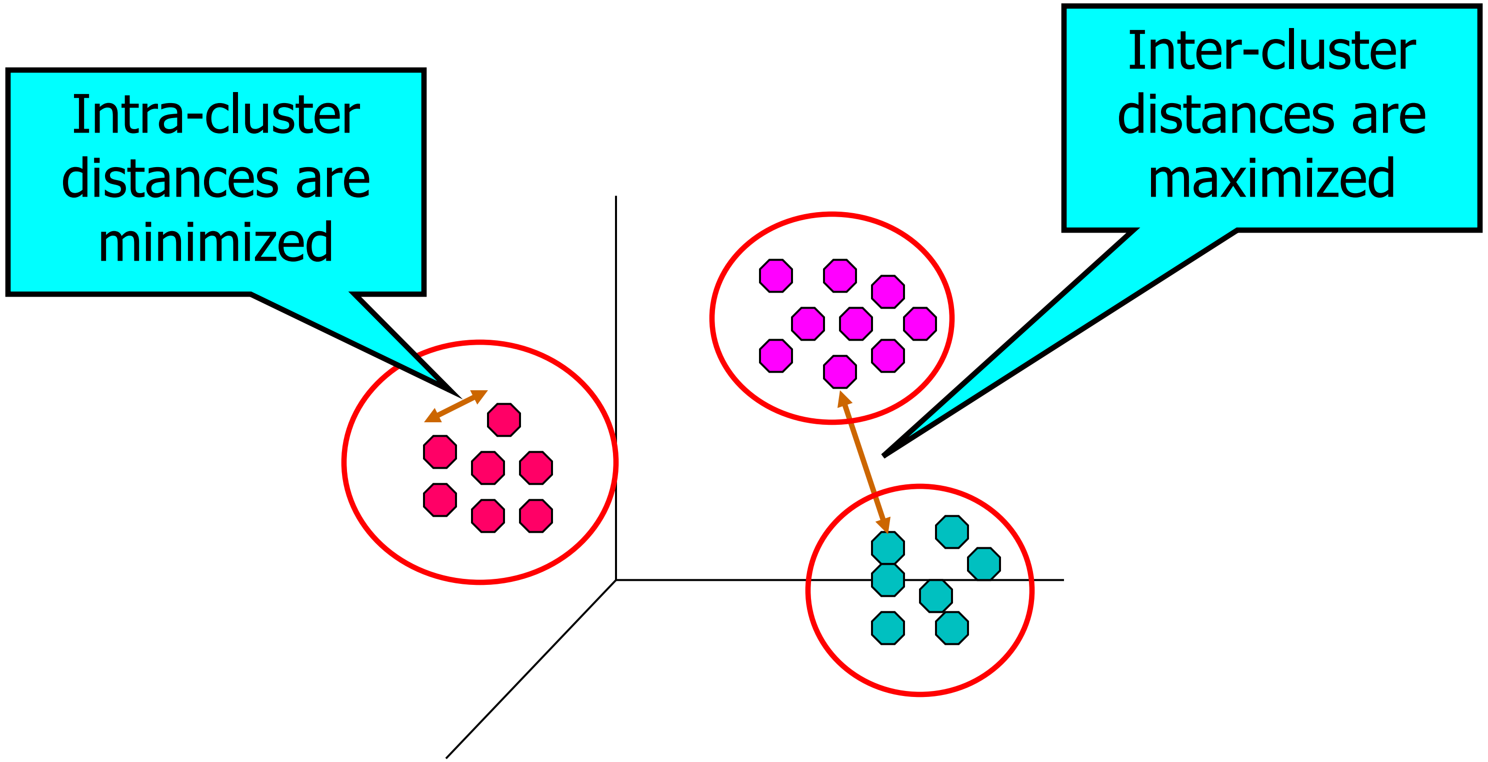
Rensselaer

What is Cluster Analysis?

- Given a set of objects, place them in groups such that the objects in a group are similar (or related) to one another and different from (or unrelated to) the objects in other groups

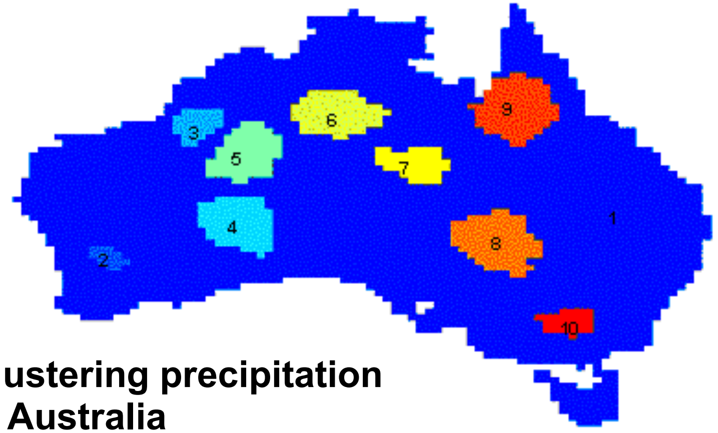


Applications of Cluster Analysis

- **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

Notion of a Cluster can be Ambiguous

How many clusters?

Six Clusters

Two Clusters

Four Clusters

Types of Clusterings

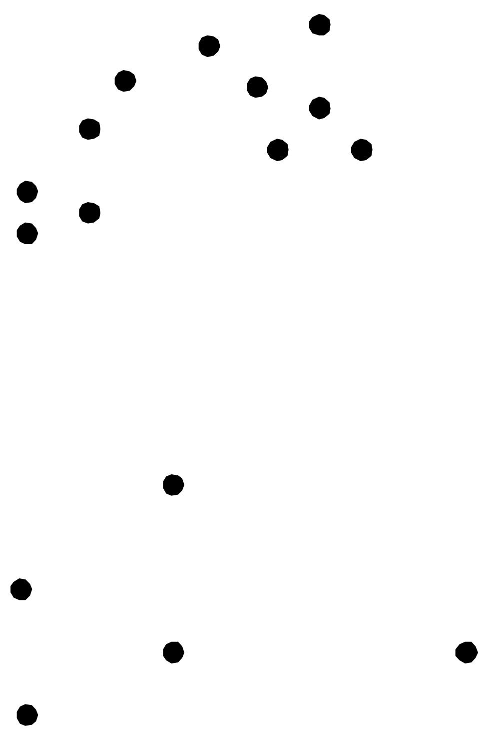
- A clustering is a set of clusters

- Important distinction between hierarchical and partitional sets of clusters

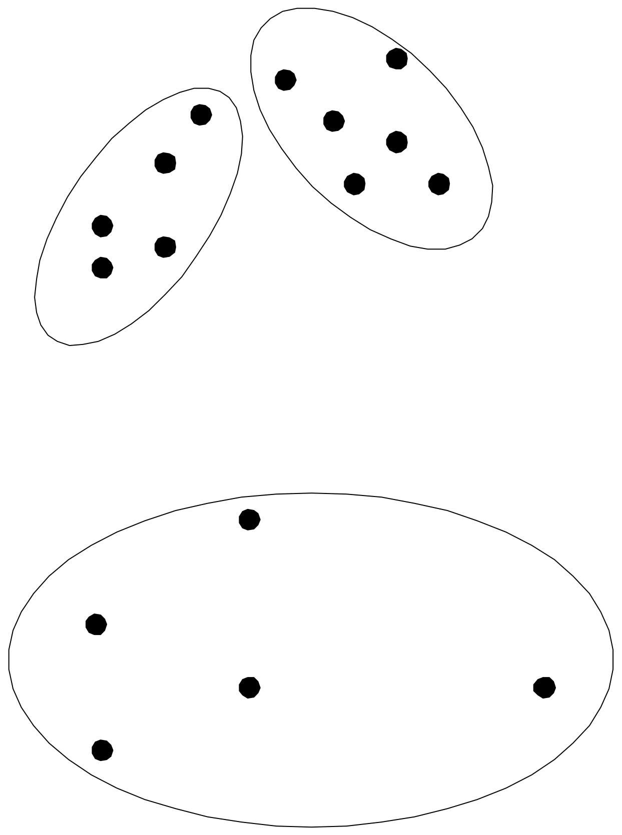
  – Partitional Clustering
    - A division of data objects into non-overlapping subsets (clusters)

  – Hierarchical clustering
    - A set of nested clusters organized as a hierarchical tree

Partitional Clustering

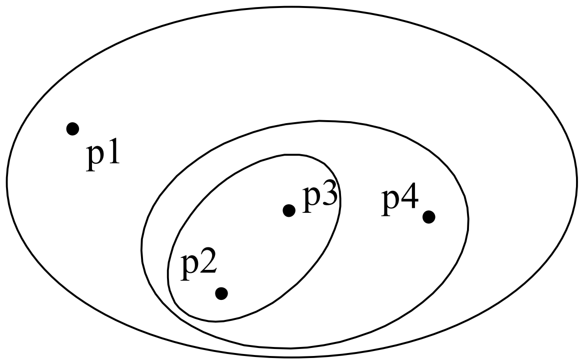


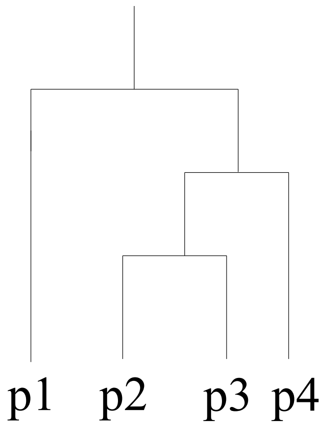
Original Points



A Partitional Clustering

Hierarchical Clustering





Other Distinctions Between Sets of Clusters

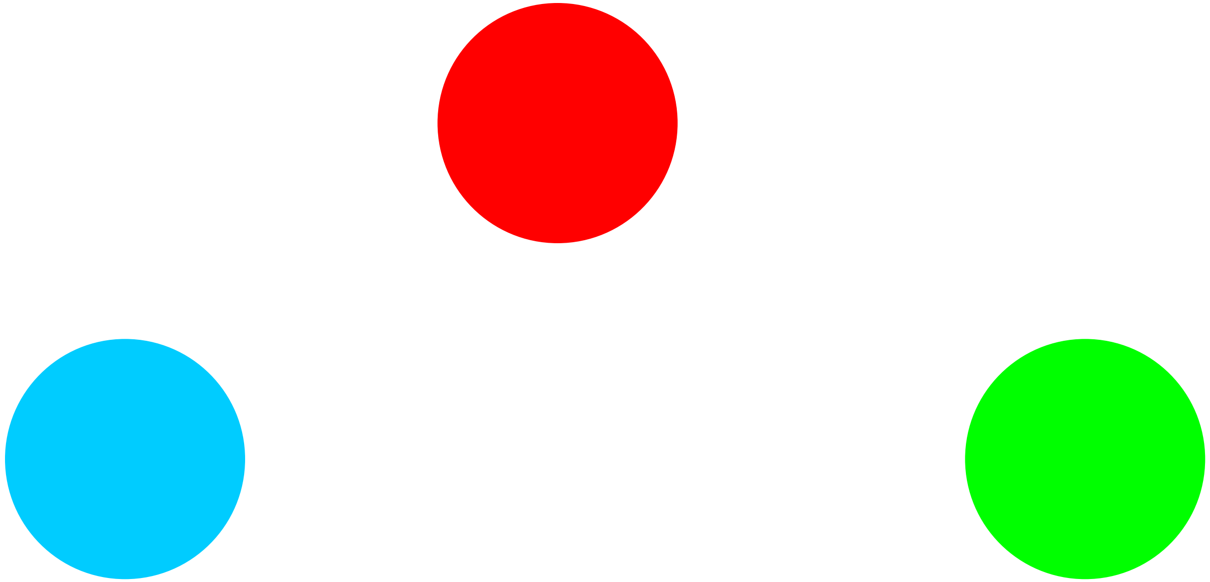
- Exclusive versus non-exclusive
  - In non-exclusive clusterings, points may belong to multiple clusters.
    - Can belong to multiple classes or could be ‘border’ points
  - Fuzzy clustering (one type of non-exclusive)
    - In fuzzy clustering, a point belongs to every cluster with some weight between 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

Types of Clusters

- Well-separated clusters
- Prototype-based clusters
- Contiguity-based clusters
- Density-based clusters
- ~~Described by an Objective Function~~

Types of Clusters: Well-Separated

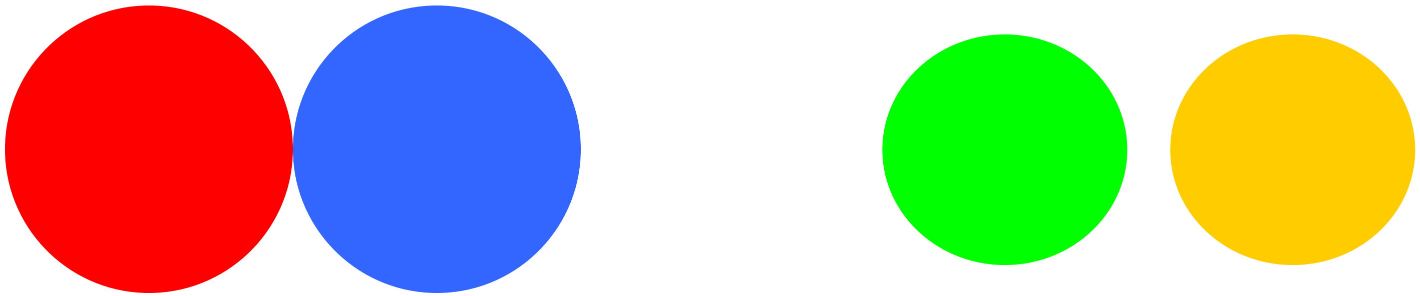
- Well-Separated Clusters:
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.



3 well-separated clusters

Types of Clusters: Prototype-Based

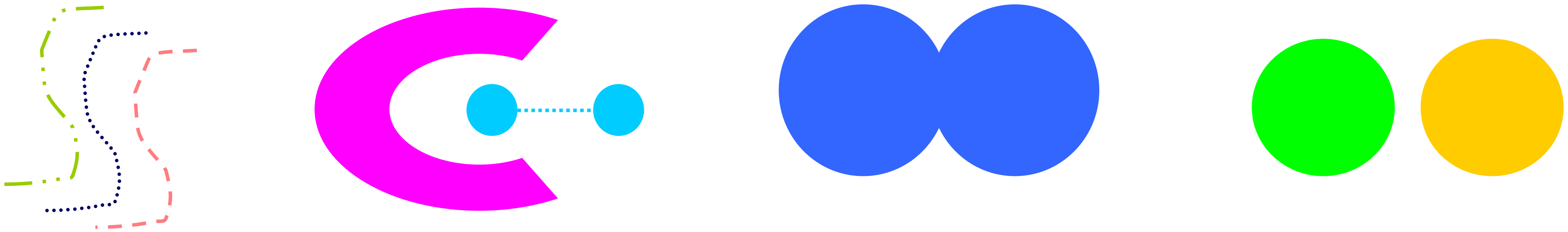
- Prototype-based
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the prototype or "center" of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the average of all the points in the cluster, or a medoid,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



4 center-based clusters

Types of Clusters: Contiguity-Based

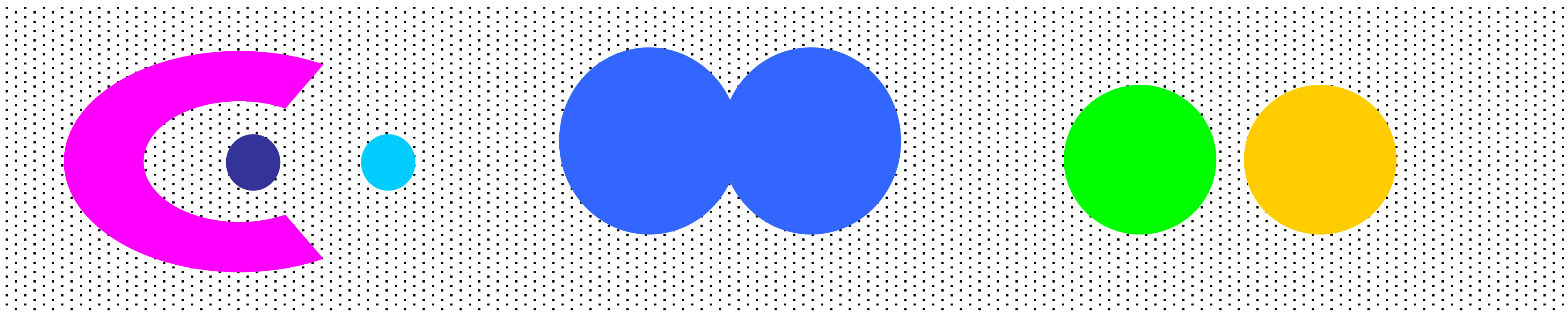
- Contiguous Cluster (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.



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

Characteristics of the Input Data Are Important

- Type of proximity or density measure
  - Central to clustering
  - Depends on data and application

- Data characteristics that affect proximity and/or density are
  - Dimensionality
    - Sparseness
  - Attribute type
  - Special relationships in the data
    - For example, autocorrelation
  - Distribution of the data

- Noise and Outliers
  - Often interfere with the operation of the clustering algorithm
- Clusters of differing sizes, densities, and shapes

Clustering Algorithms

- K-means and its variants

- Hierarchical clustering

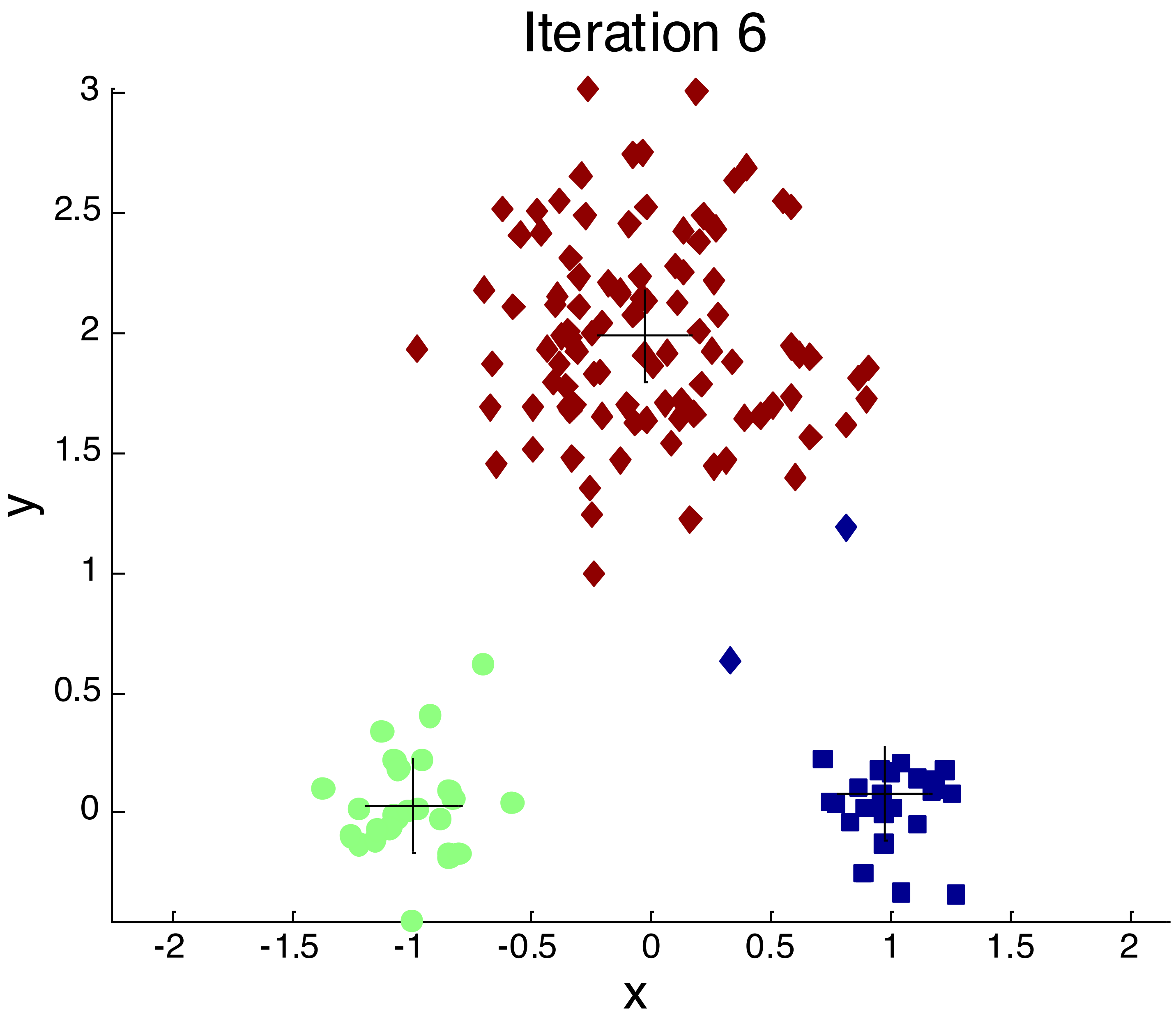
- ~~Density-based clustering~~

K-means Clustering

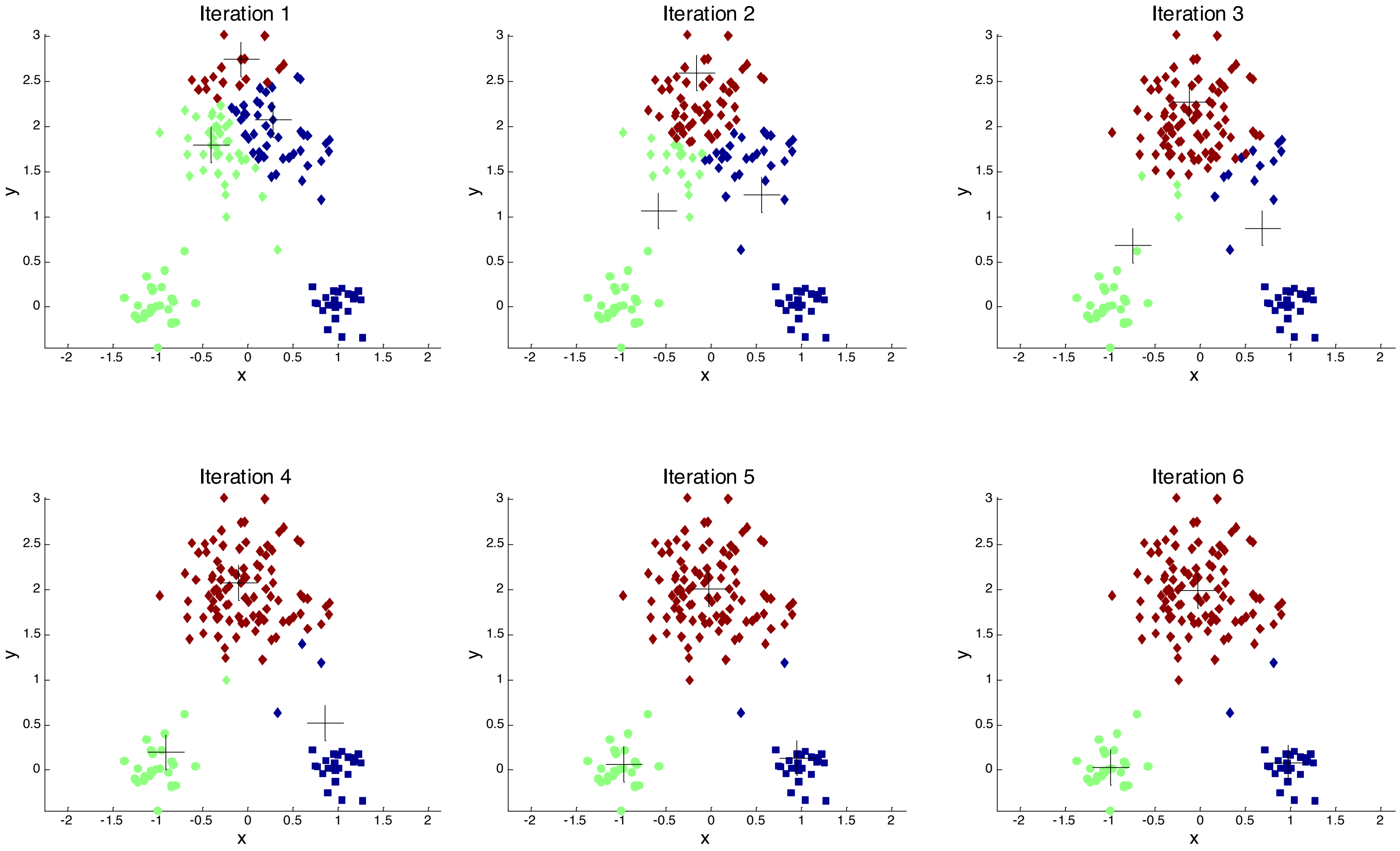
- Partitional clustering approach
- Number of clusters, K, must be specified
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid
- The basic algorithm is very simple

1: Select K points as the initial centroids.
2: **repeat**
3:     Form K clusters by assigning all points to the closest centroid.
4:     Recompute the centroid of each cluster.
5: **until** The centroids don't change

Example of K-means Clustering



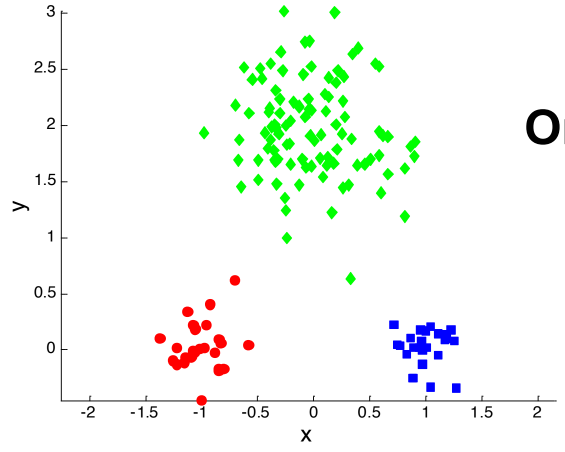
Example of K-means Clustering



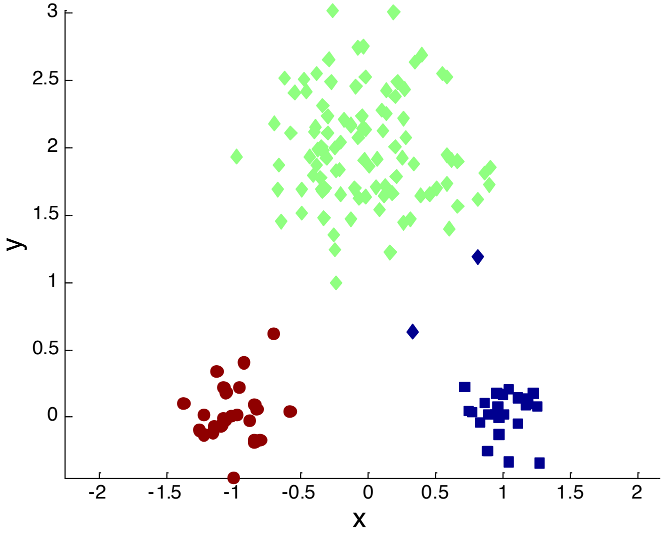
K-means Clustering – Details

- Simple iterative algorithm.
  - Choose initial centroids;
  - repeat {assign each point to a nearest centroid; re-compute cluster centroids}
  - until centroids stop changing.
- Initial centroids are often chosen randomly.
  - Clusters produced can vary from one run to another
- The centroid is (typically) the mean of the points in the cluster, but other definitions are possible.
- K-means will converge for common proximity measures with appropriately defined centroid
- Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to 'Until relatively few points change clusters'

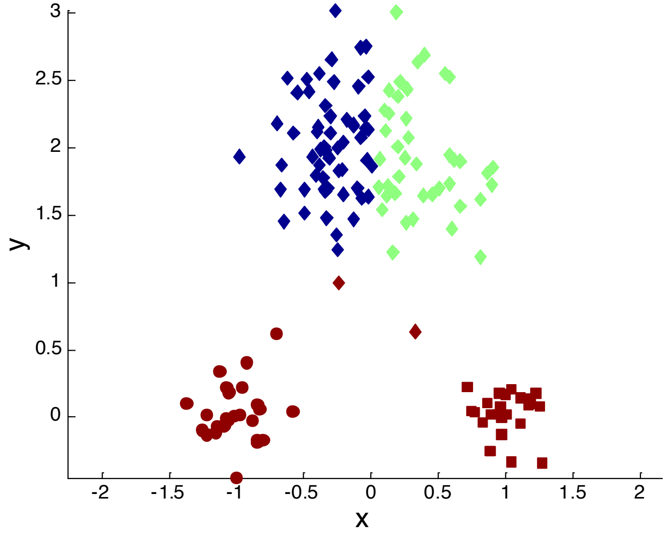
Two different K-means Clusterings



Original Points

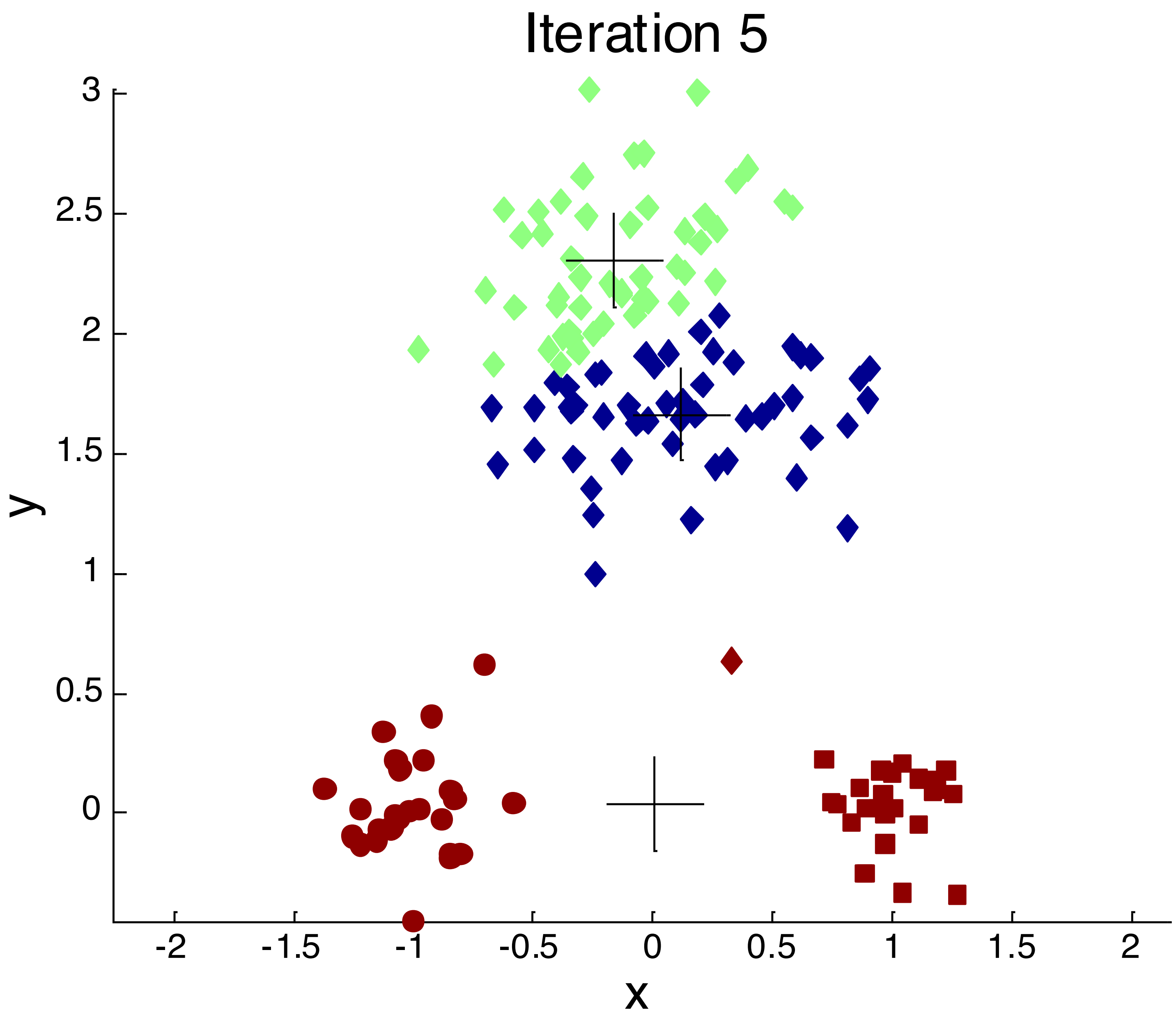


Optimal Clustering

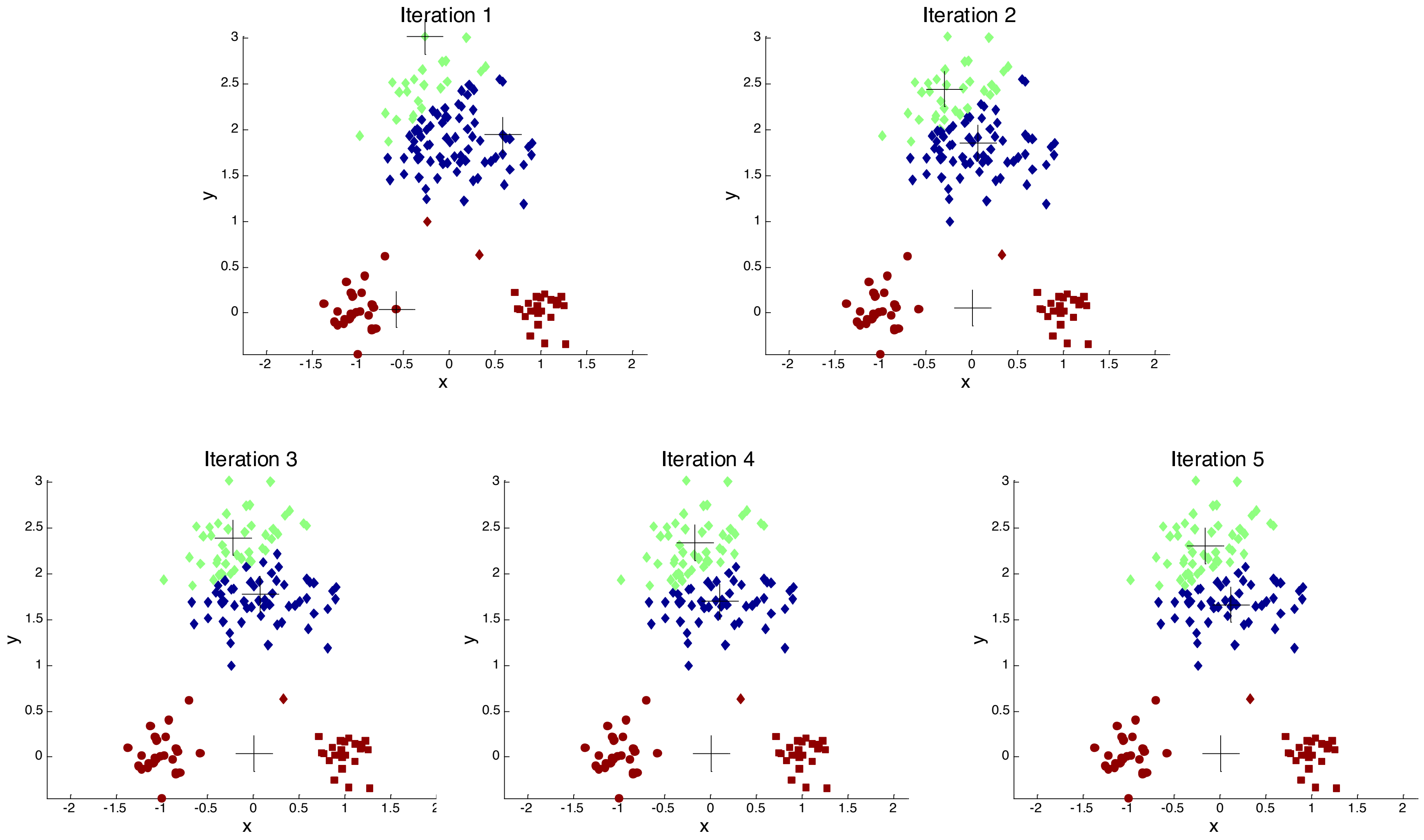


Sub-optimal Clustering

Importance of Choosing Initial Centroids …

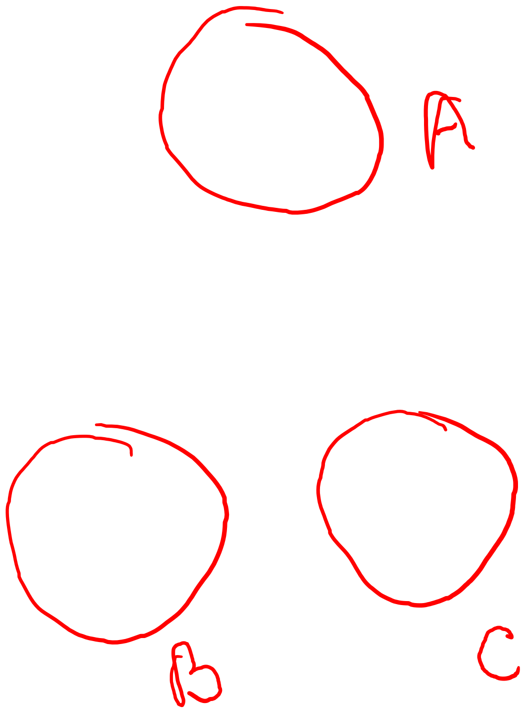


Importance of Choosing Initial Centroids …



Importance of Choosing Intial Centroids

- Depending on the choice of initial centroids, B and C may get merged or remain separate



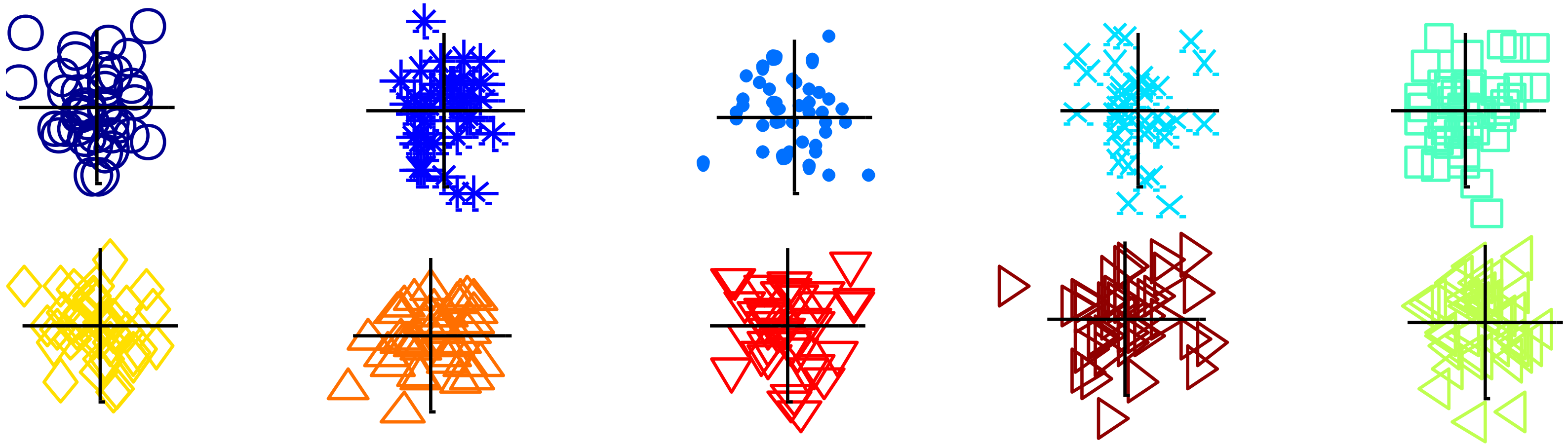
Problems with Selecting Initial Points

- 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

$$P = \frac{\text{number of ways to select one centroid from each cluster}}{\text{number of ways to select } K \text{ centroids}} = \frac{K!n^K}{(Kn)^K} = \frac{K!}{K^K}$$

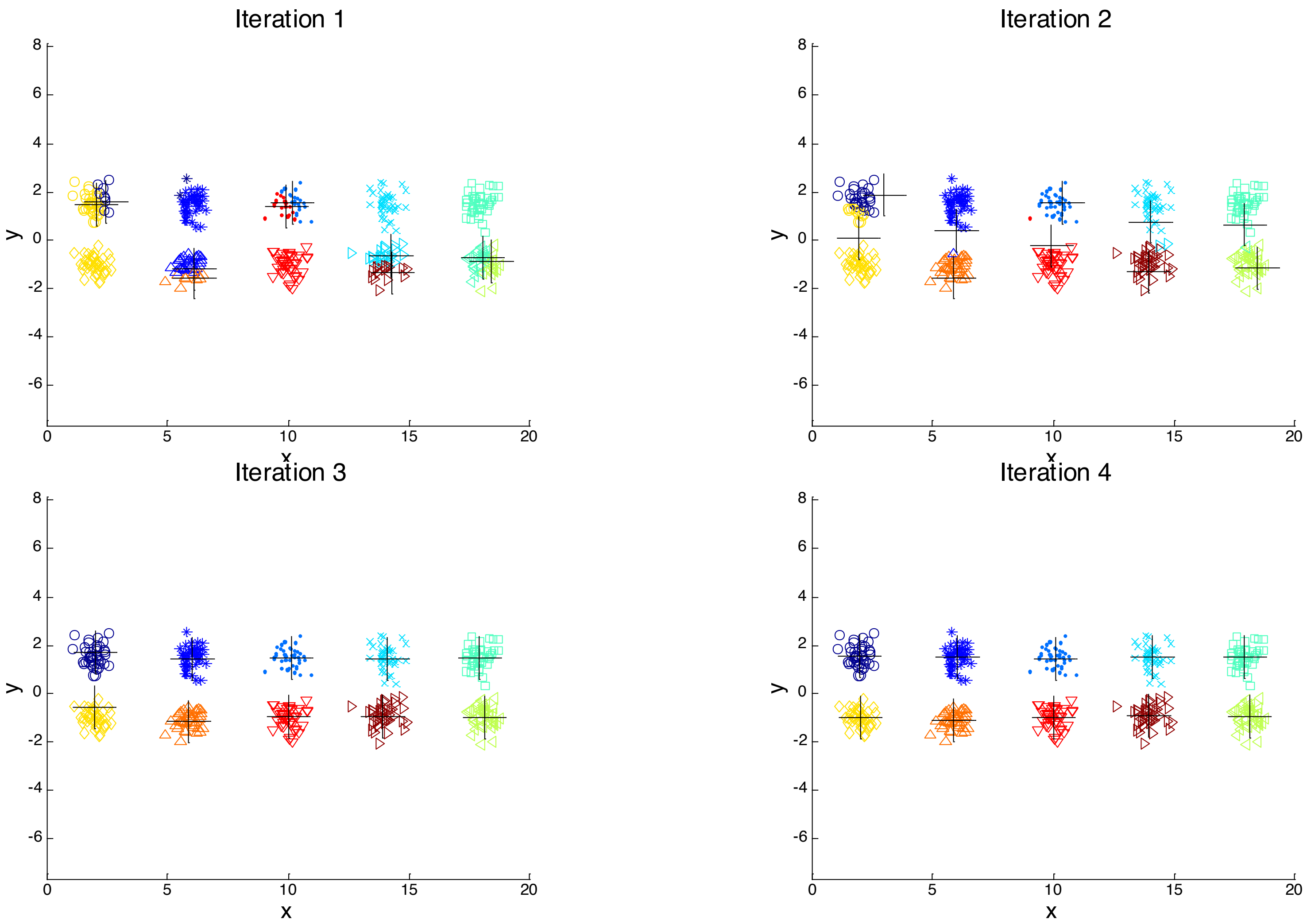
  - For example, if K = 10, then probability = $10!/10^{10}$ = 0.00036
  - Sometimes the initial centroids will readjust themselves in 'right' way, and sometimes they don't
  - Consider an example of five pairs of clusters

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

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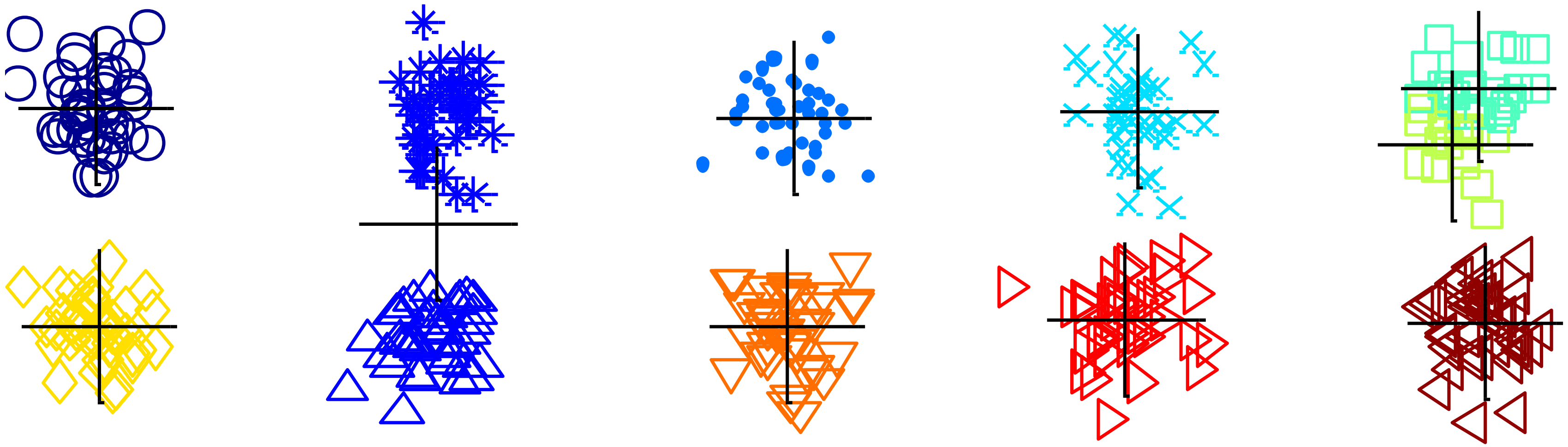
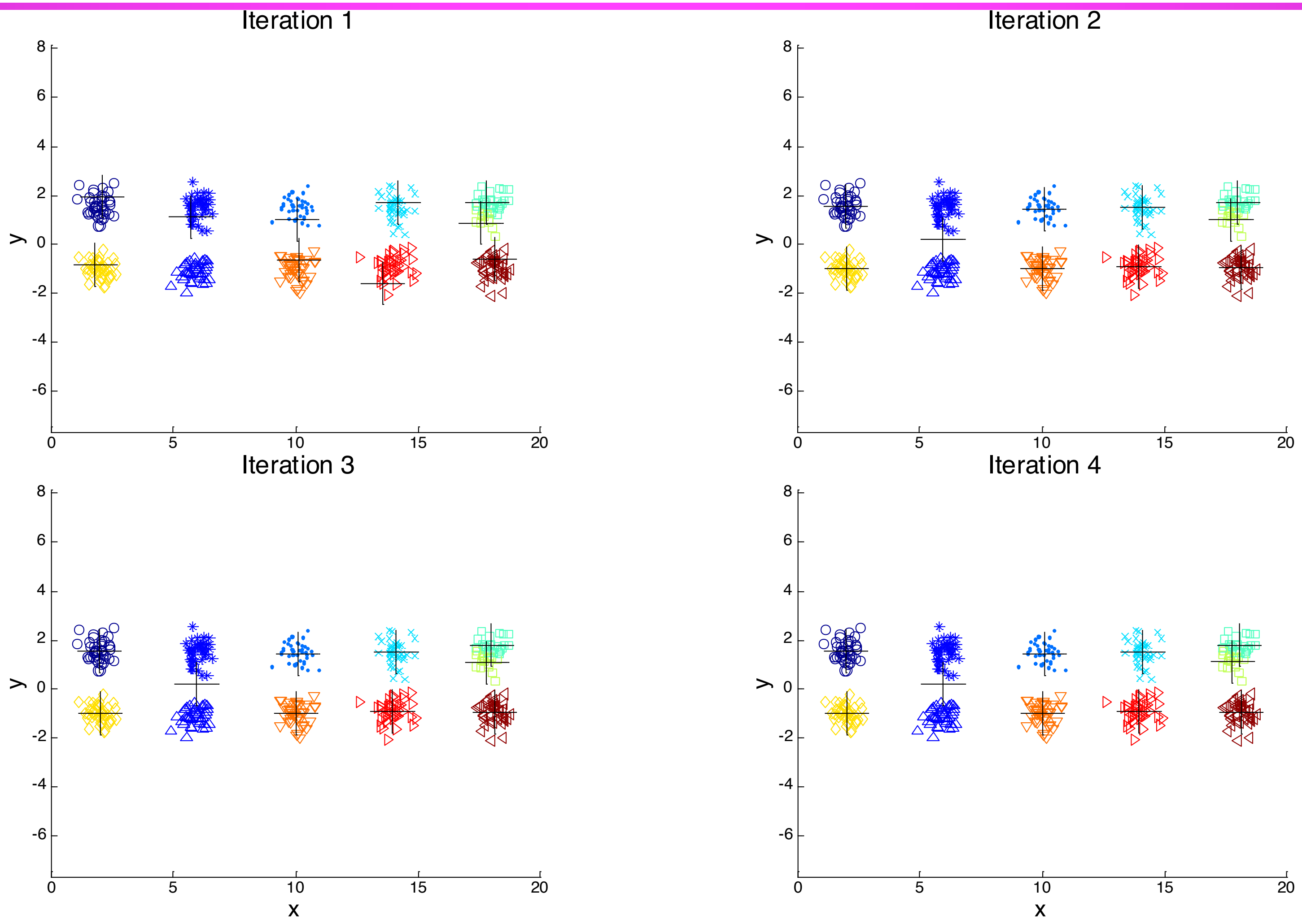


Starting with some pairs of clusters having three initial centroids, while other have only one.

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
- Use some strategy to select the k initial centroids and then select among these initial centroids
  - Select most widely separated
    - K-means++ is a robust way of doing this selection
  - Use hierarchical clustering to determine initial centroids
- ~~Bisecting K-means~~
  - ~~Not as susceptible to initialization issues~~

K-means++

- This approach can be slower than random initialization, but very consistently produces better results in terms of SSE
  – The k-means++ algorithm guarantees an approximation ratio O(log k) in expectation, where k is the number of centers
- To select a set of initial centroids, *C*, perform the following

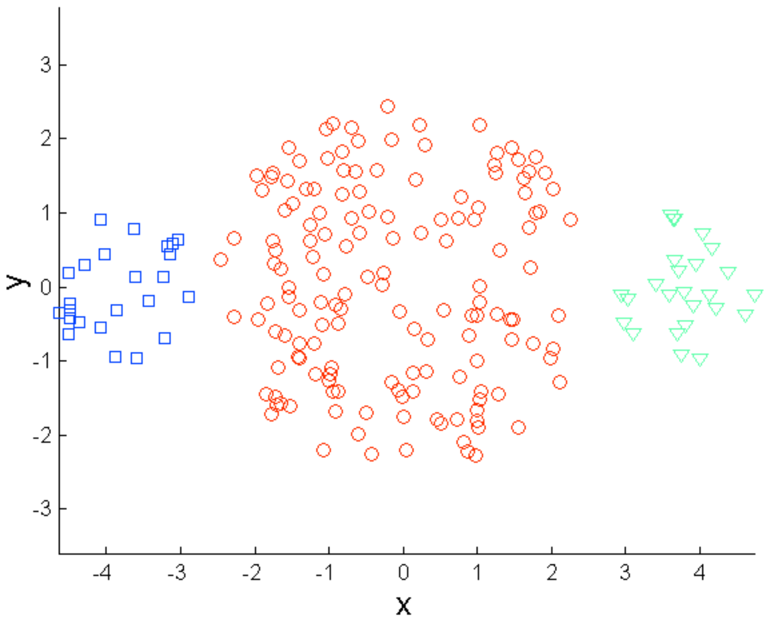
1. Select an initial point at random to be the first centroid
2. For k – 1 steps
3. For each of the N points, x_i, $1 \le i \le N$, find the minimum squared distance to the currently selected centroids, $C_1, \ldots, C_j$, $1 \le j < k$, i.e., $\min_j d^2(C_j, x_i)$
4. Randomly select a new centroid by choosing a point with probability proportional to $\frac{\min_j d^2(C_j, x_i)}{\sum_i \min_j d^2(C_j, x_i)}$ is
5. End For

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.
  - One possible solution is to remove outliers before clustering

Limitations of K-means: Differing Sizes



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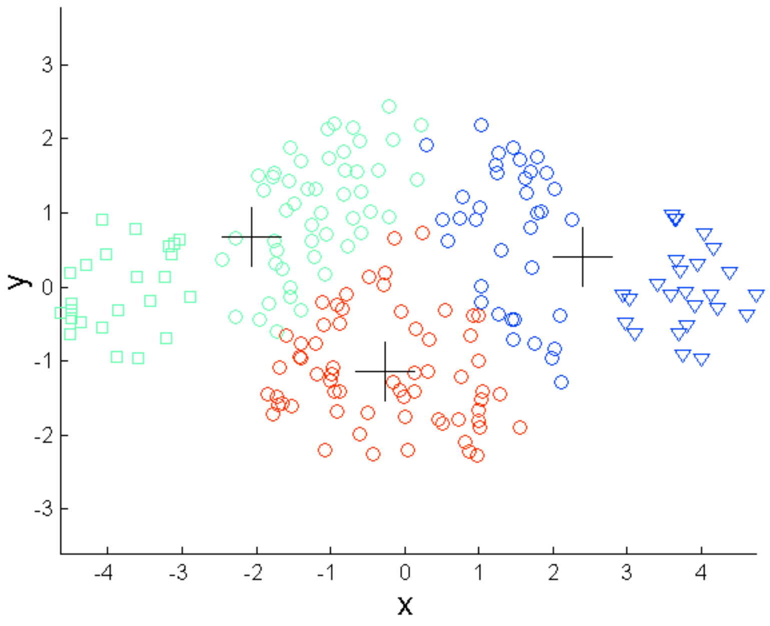
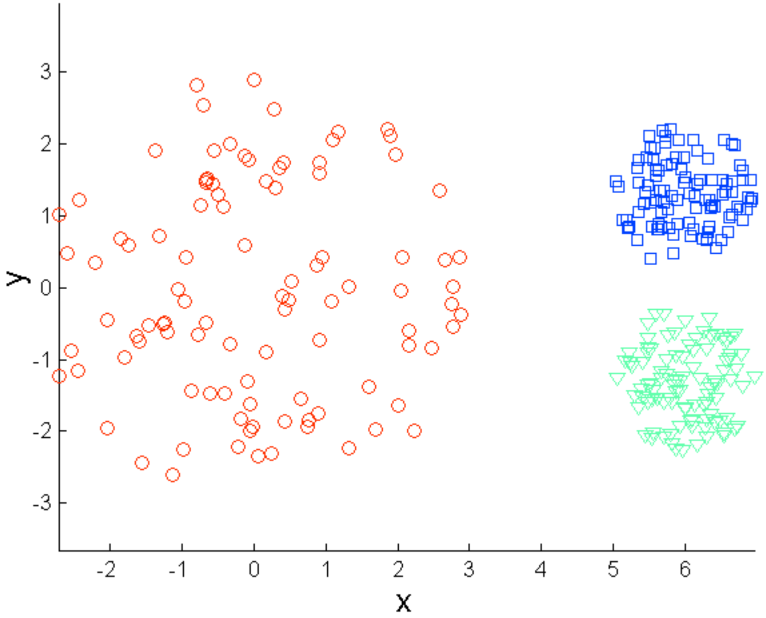
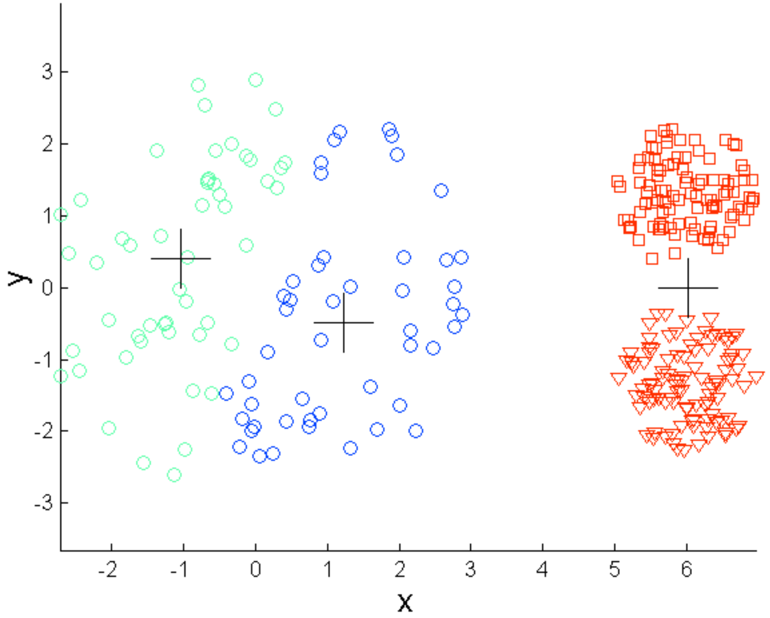


K-means (3 Clusters)

Limitations of K-means: Differing Density

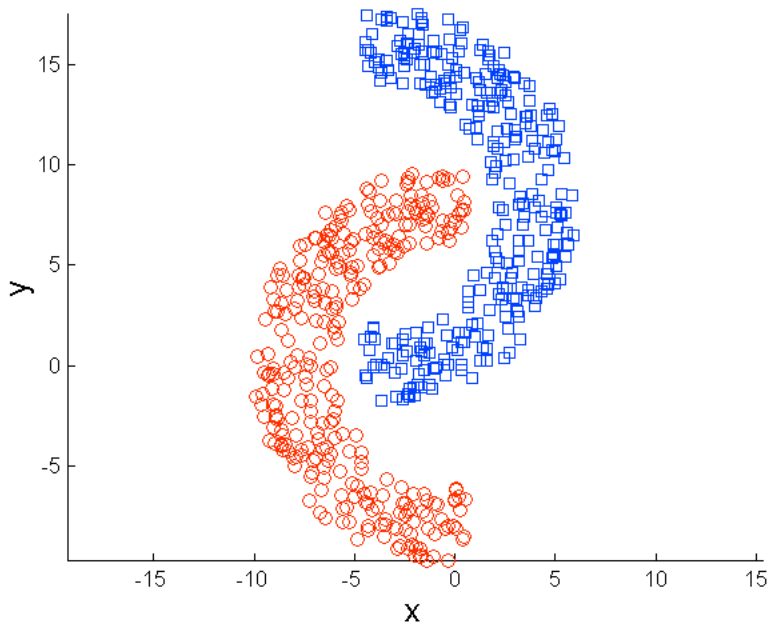


Original Points



K-means (3 Clusters)

Limitations of K-means: Non-globular Shapes



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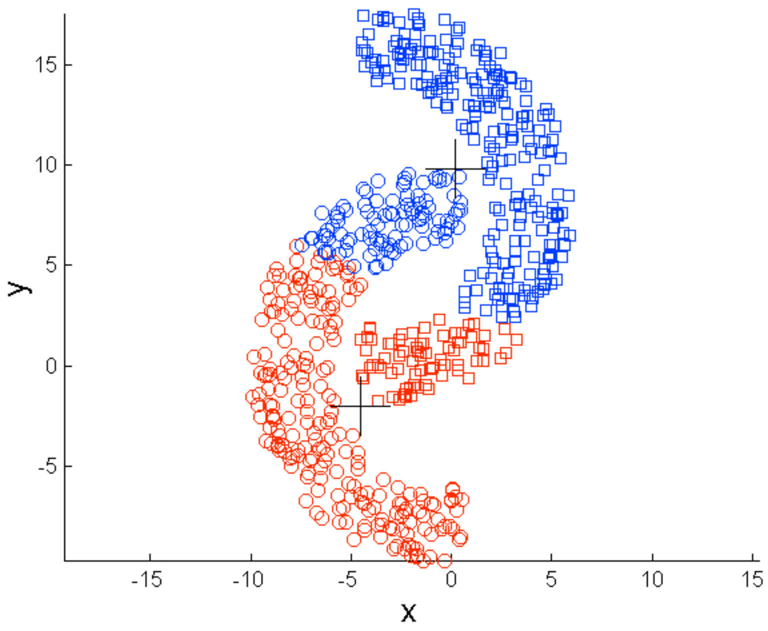
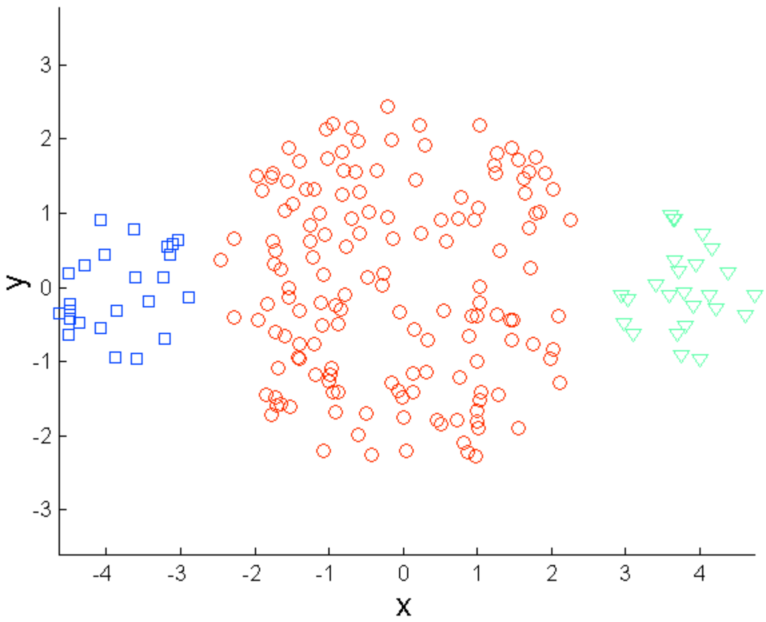


K-means (2 Clusters)

Overcoming K-means Limitations



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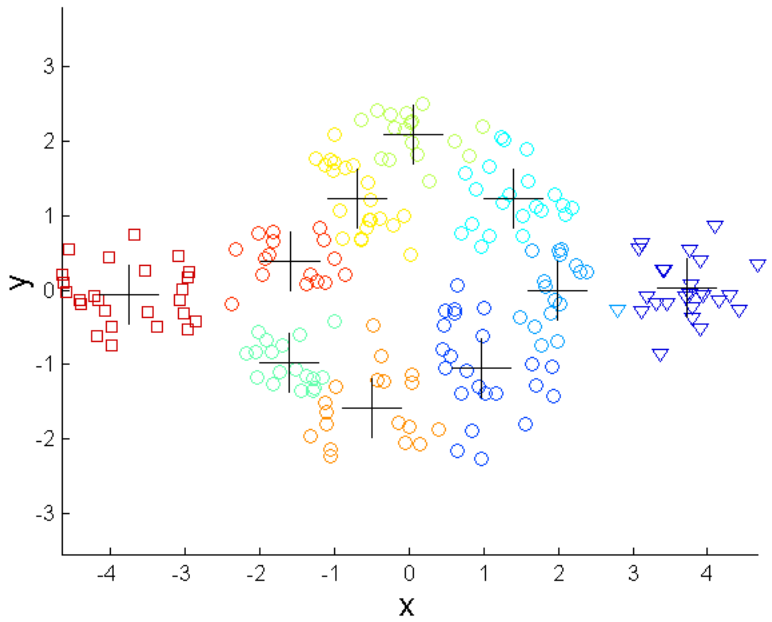
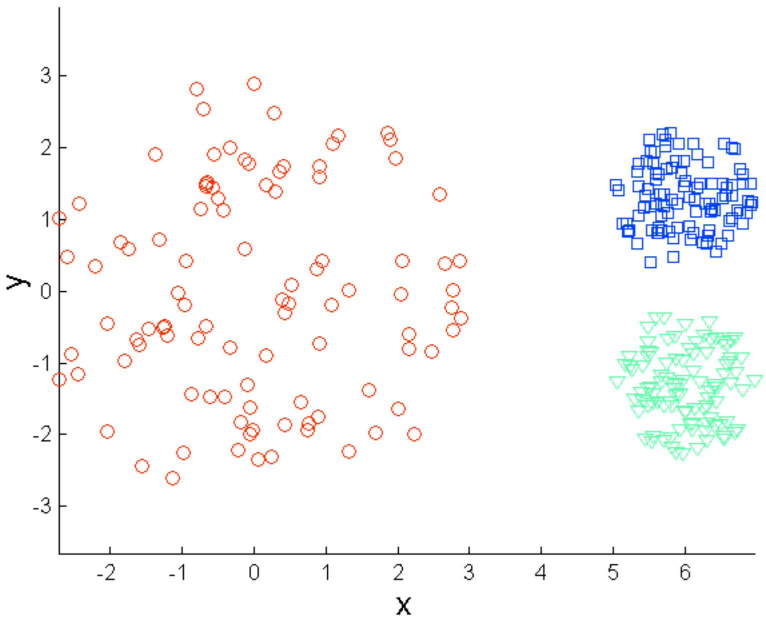


K-means Clusters

One solution is to find a large number of clusters such that each of them represents a part of a natural cluster. But these small clusters need to be put together in a post-processing step.

Overcoming K-means Limitations



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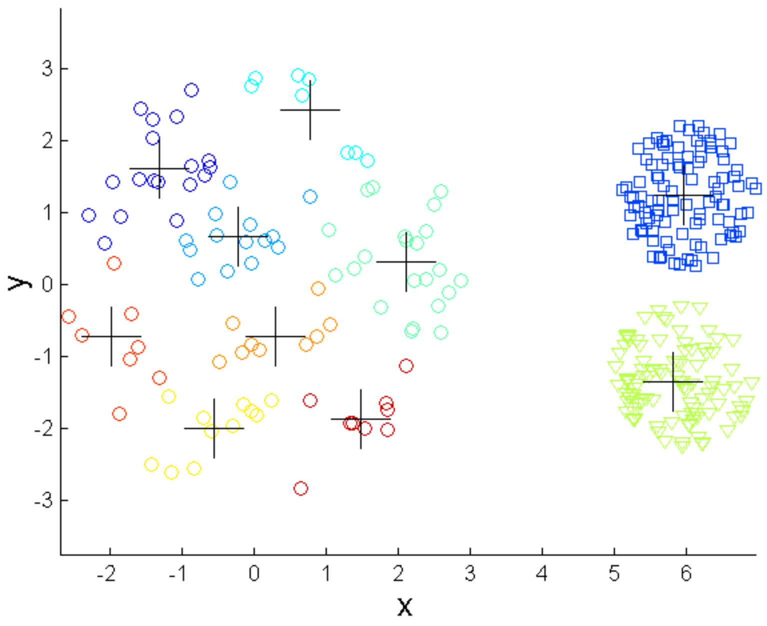

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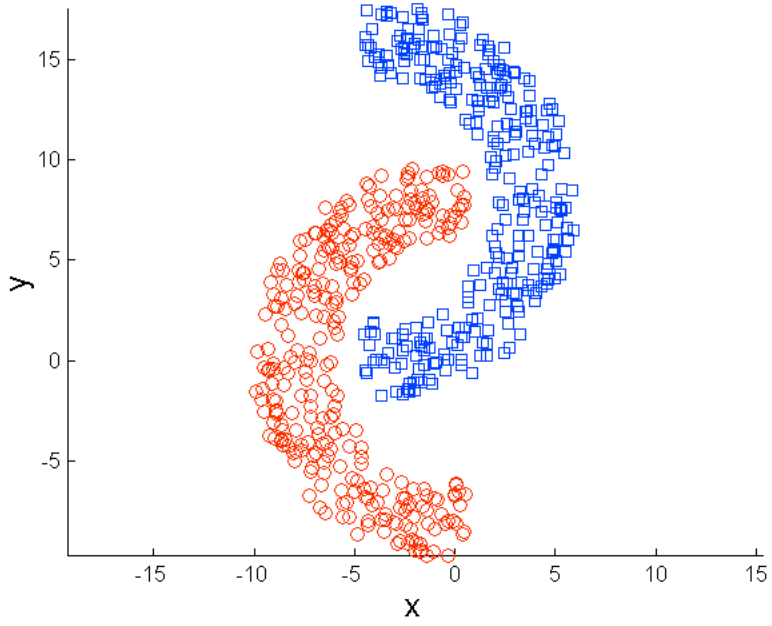

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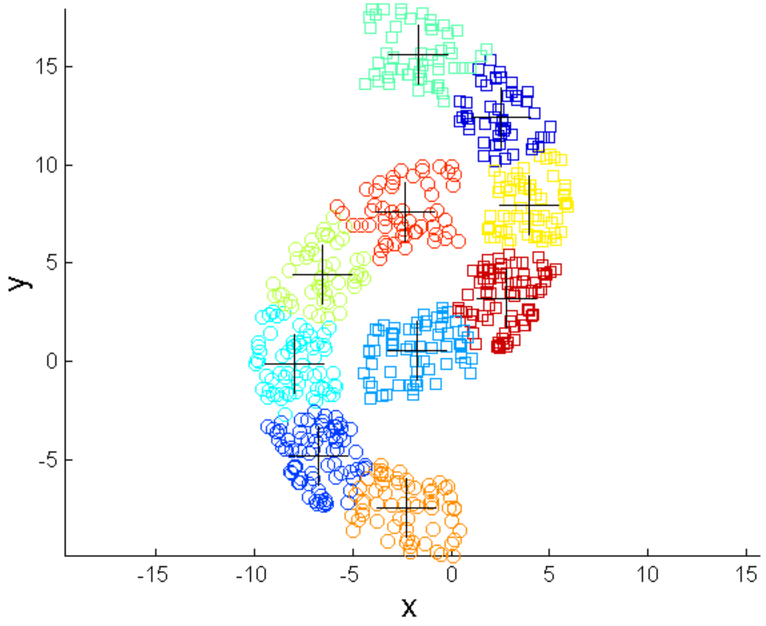
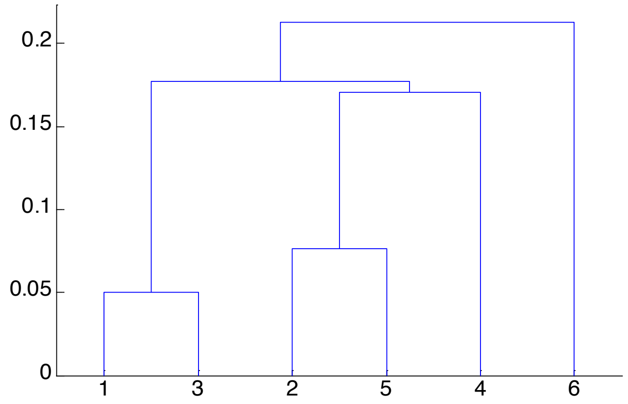


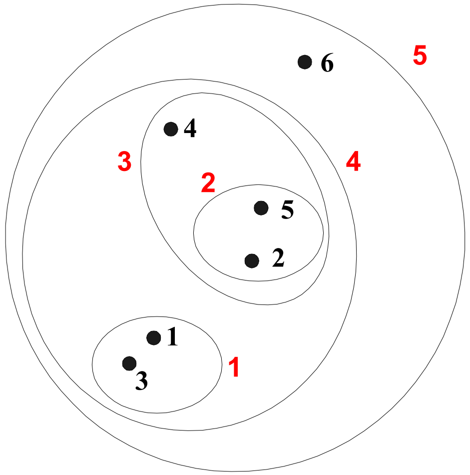
K-means Clusters

One solution is to find a large number of clusters such that each of them represents a part of a natural cluster. But these small clusters need to be put together in a post-processing step.

Hierarchical Clustering

- Produces a set of nested clusters organized as a hierarchical tree
- Can be visualized as a dendrogram
  - A tree like diagram that records the sequences of merges or splits





Strengths of Hierarchical Clustering

- Do not have to assume any particular number of clusters
  - Any desired number of clusters can be obtained by ‘cutting’ the dendrogram at the proper level

- They may correspond to meaningful taxonomies
  - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, …)

Hierarchical Clustering

- Two main types of hierarchical clustering
  - Agglomerative (bottom-up):
    - Start with the points as individual clusters
    - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
  - Divisive (top-down):
    - Start with one, all-inclusive cluster
    - At each step, split a cluster until each cluster contains an individual point (or there are k clusters)
- Traditional hierarchical algorithms use a similarity or distance matrix
  - Merge or split one cluster at a time

Cluster Validity

- For supervised classification we have a variety of measures to evaluate how good our model is
  - Accuracy, precision, recall

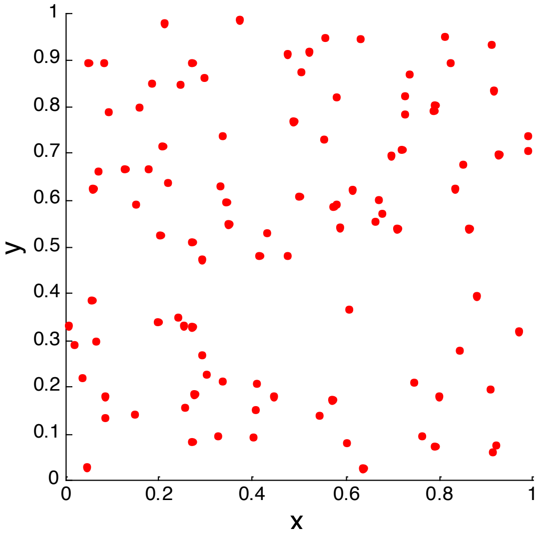
- For cluster analysis, the analogous question is how to evaluate the "goodness" of the resulting clusters?

- But "clusters are in the eye of the beholder"!
  - In practice the clusters we find are defined by the clustering algorithm

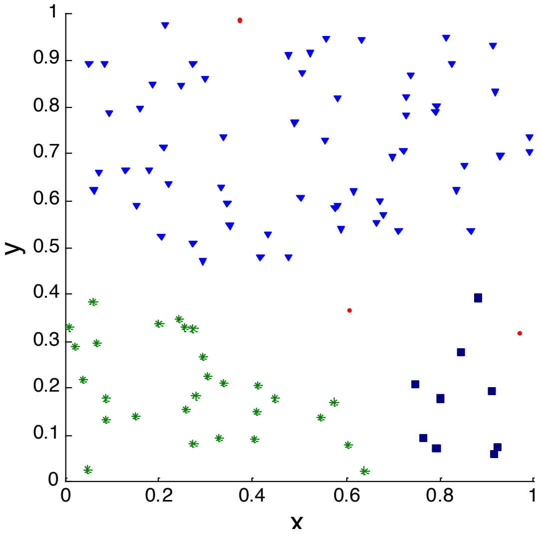
- Then why do we want to evaluate them?
  - To avoid finding patterns in noise
  - To compare clustering algorithms
  - To compare two sets of clusters
  - To compare two clusters

Clusters found in Random Data

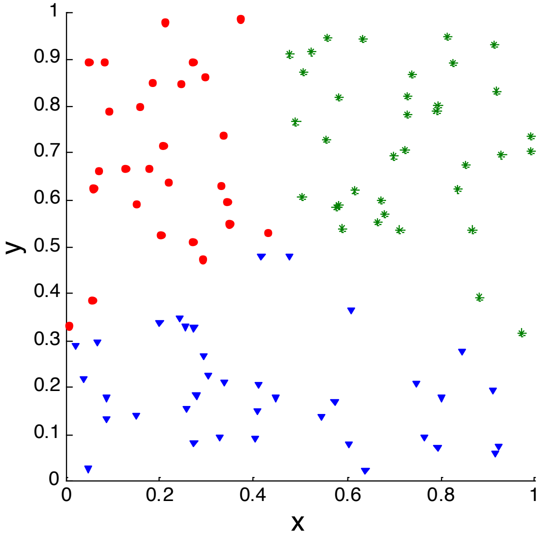
Random Points



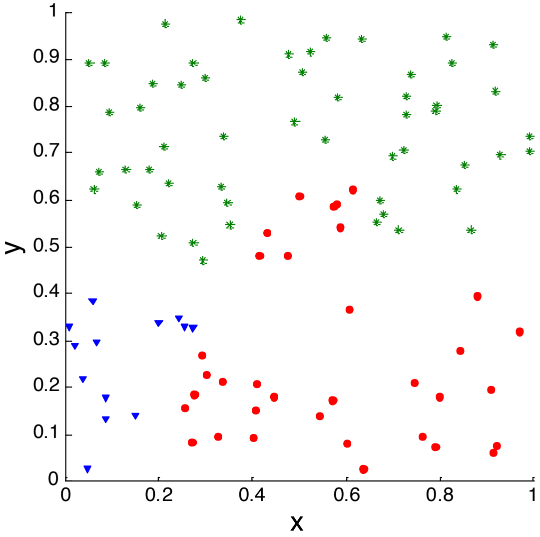
DBSCAN



K-means



Complete Link



Measures of Cluster Validity

- Numerical measures that are applied to judge various aspects of cluster validity, are classified into the following two types.
  - Supervised: Used to measure the extent to which cluster labels match externally supplied class labels.
    - Entropy
    - Often called *external indices* because they use information external to the data
  - Unsupervised: Used to measure the goodness of a clustering structure *without* respect to external information.
    - Sum of Squared Error (SSE)
    - Often called *internal indices* because they only use information in the data

- You can use supervised or unsupervised measures to compare clusters or clusterings

K-means Objective Function

- A common objective function (used with Euclidean distance measure) is Sum of Squared Error (SSE)
  - For each point, the error is the distance to the nearest cluster center
  - 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 centroid (mean) for cluster C_i
  - SSE improves in each iteration of K-means until it reaches a local or global minima.
  - This is called the model's inertia: the mean squared distance between each instance and its closest centroid.

Unsupervised Measures: Cohesion and Separation

- Cluster Cohesion: Measures how closely related are objects in a cluster
  - Example: SSE
- Cluster Separation: Measure how distinct or well-separated a cluster is from other clusters
- Example: Squared Error
  - Cohesion is measured by the within cluster sum of squares (SSE)

$$SSE = \sum_{i} \sum_{x \in C_i} (x - m_i)^2$$

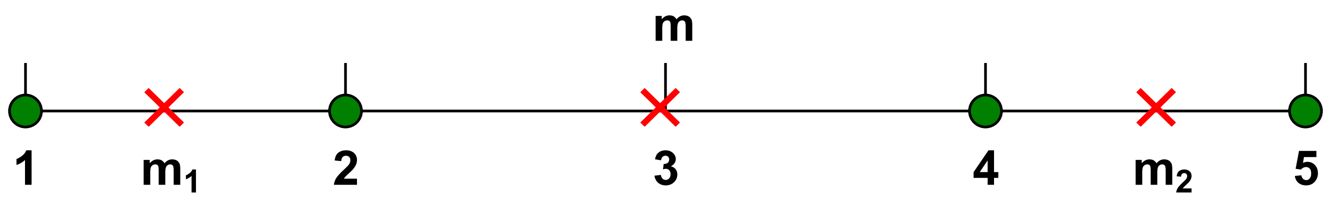
  - Separation is measured by the between cluster sum of squares

$$SSB = \sum_{i} |C_i| (m - m_i)^2$$

Where $|C_i|$ is the size of cluster *i*, *m* is the global average point, m_i is the centroid of cluster *i*, and *x* is a point in the cluster

Unsupervised Measures: Cohesion and Separation

- Example: SSE
  - SSB + SSE = constant



K=1 cluster:

$$SSE = (1-3)^2 + (2-3)^2 + (4-3)^2 + (5-3)^2 = 10$$
$$SSB = 4\times(3-3)^2 = 0$$
$$Total = 10 + 0 = 10$$

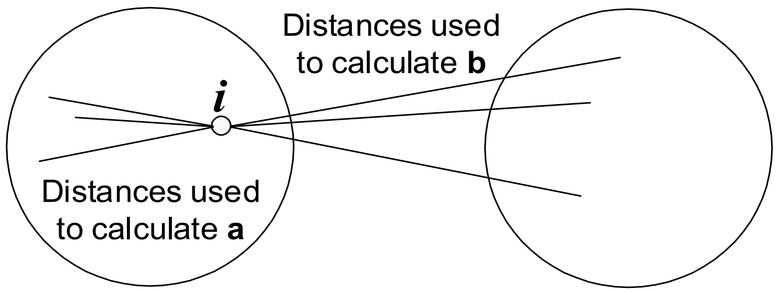
K=2 clusters:

$$SSE = (1-1.5)^2 + (2-1.5)^2 + (4-4.5)^2 + (5-4.5)^2 = 1$$
$$SSB = 2\times(3-1.5)^2 + 2\times(4.5-3)^2 = 9$$
$$Total = 1 + 9 = 10$$

Unsupervised Measures: Silhouette Coefficient

- Silhouette coefficient combines ideas of both cohesion and separation, but for individual points, as well as clusters and clusterings
- For an individual point, ***i***
  - Calculate ***a*** = average distance of ***i*** to the points in its cluster
  - Calculate ***b*** = min (average distance of ***i*** to points in another cluster)
  - The silhouette coefficient for a point is then given by

    s = (b – a) / max(a,b)

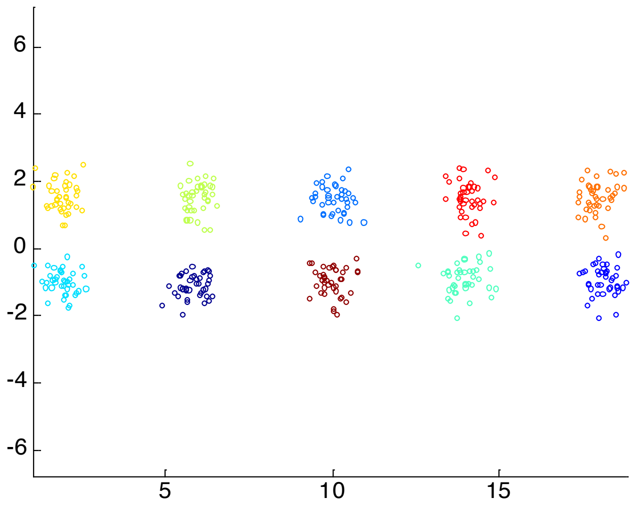


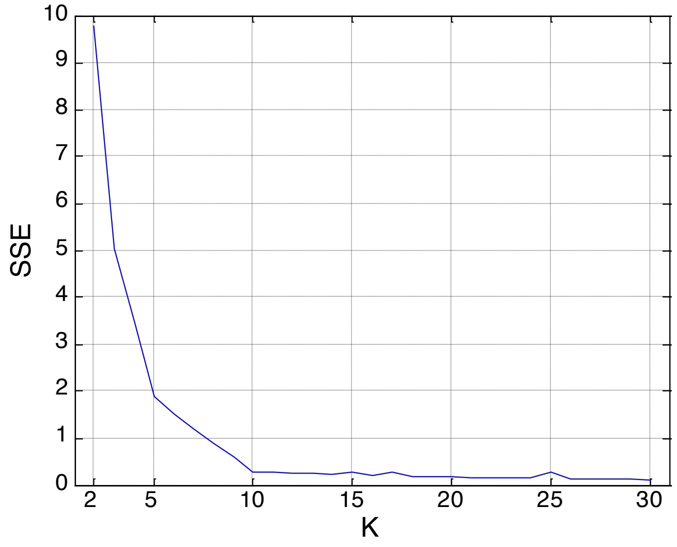
  - Value can vary between -1 and 1
  - Typically ranges between 0 and 1.
  - The closer to 1 the better.

- Can calculate the average silhouette coefficient for a cluster or a clustering

Determining the Correct Number of Clusters

- SSE is good for comparing two clusterings or two clusters
- SSE can also be used to estimate the number of clusters





Selecting the Number of Clusters

Can use the elbow method of inertia, similar to elbow method of PCA.

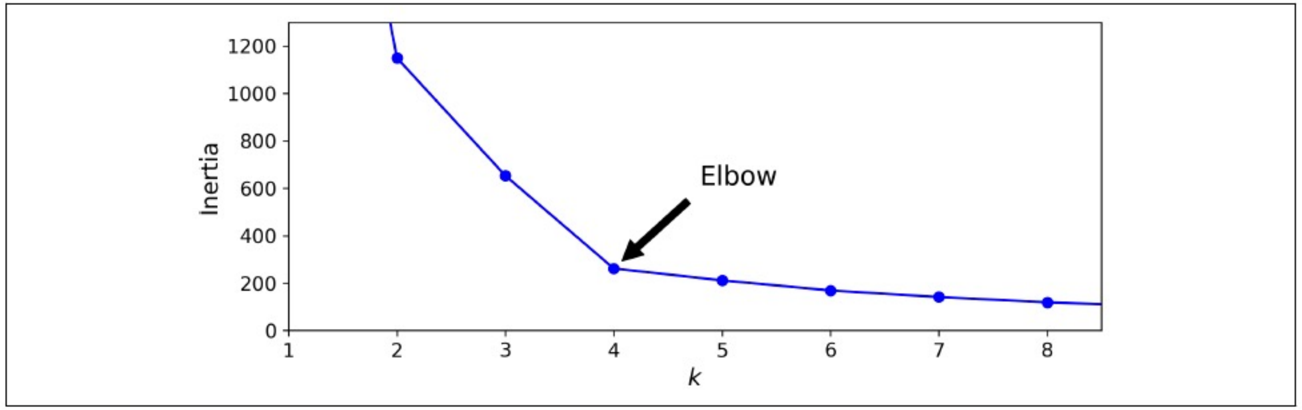
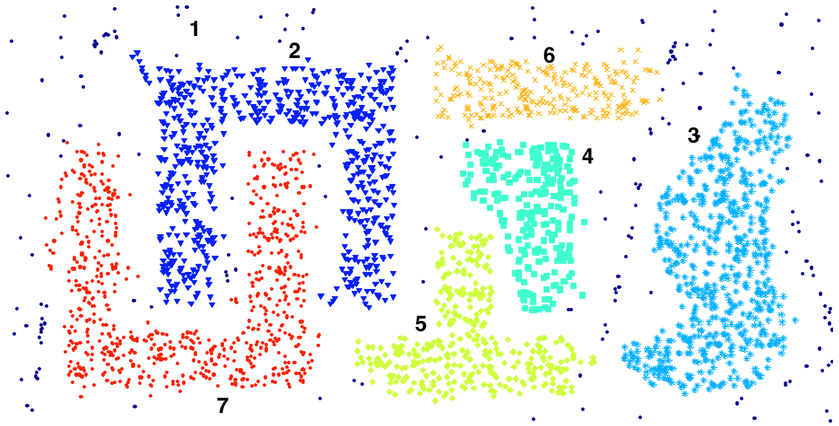
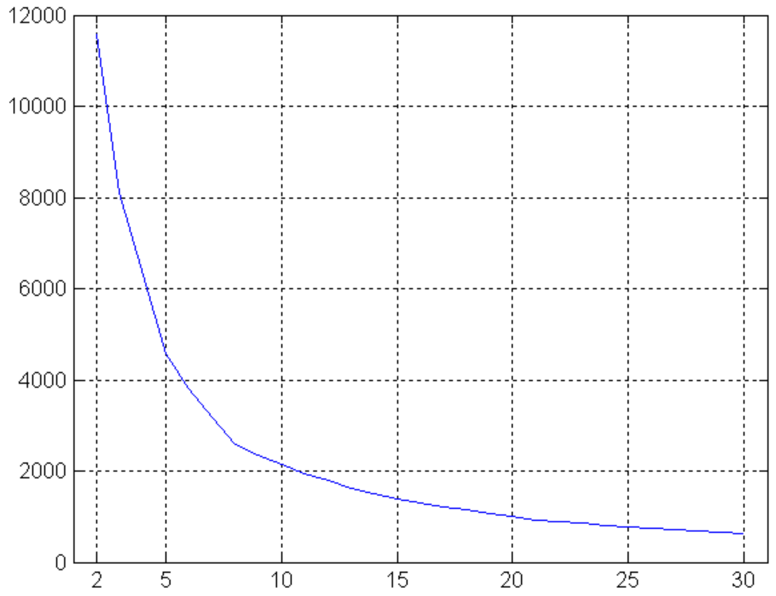


Figure 9-8. Selecting the number of clusters k using the "elbow rule"

Determining the Correct Number of Clusters

- SSE curve for a more complicated data set





SSE of clusters found using K-means