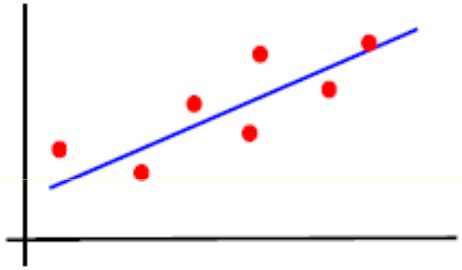
Unsupervised Learning : Clustering

Things to be Addressed

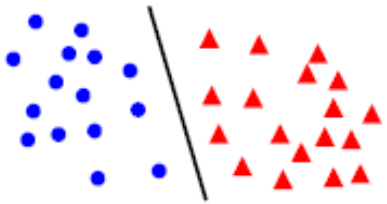
- Traditional Learning Models.
- Cluster Analysis
- K-means Clustering Algorithm
- Drawbacks of traditional clustering algorithms.
- Clustering as a complex multi-modal optimization problem.

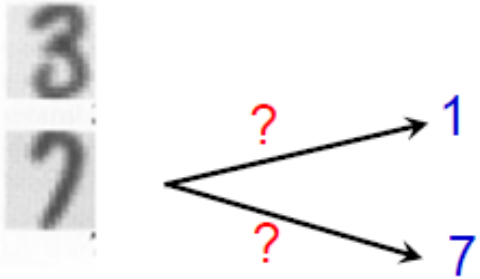
Three canonical learning problems

1. Regression - supervised
   - estimate parameters, e.g. of weight vs height



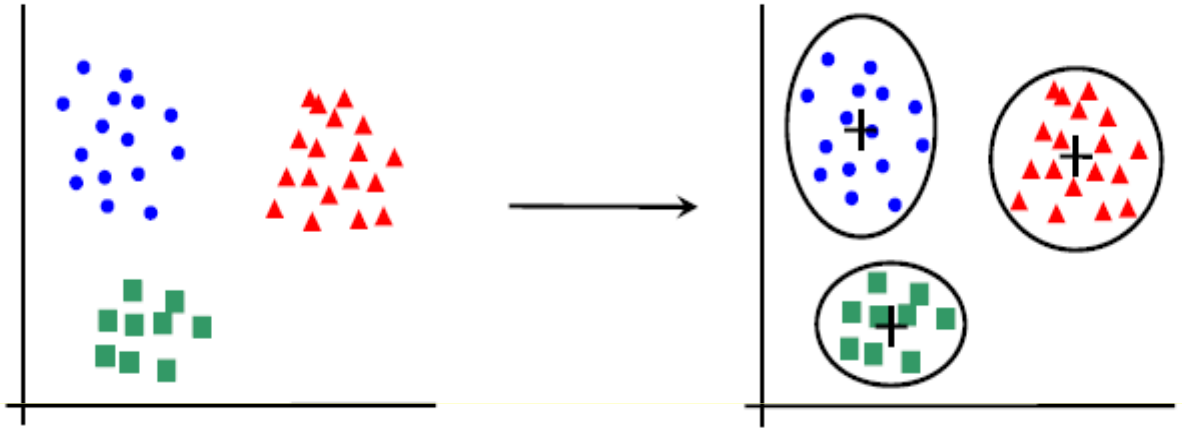
2. Classification - supervised
   - estimate class, e.g. handwritten digit classification



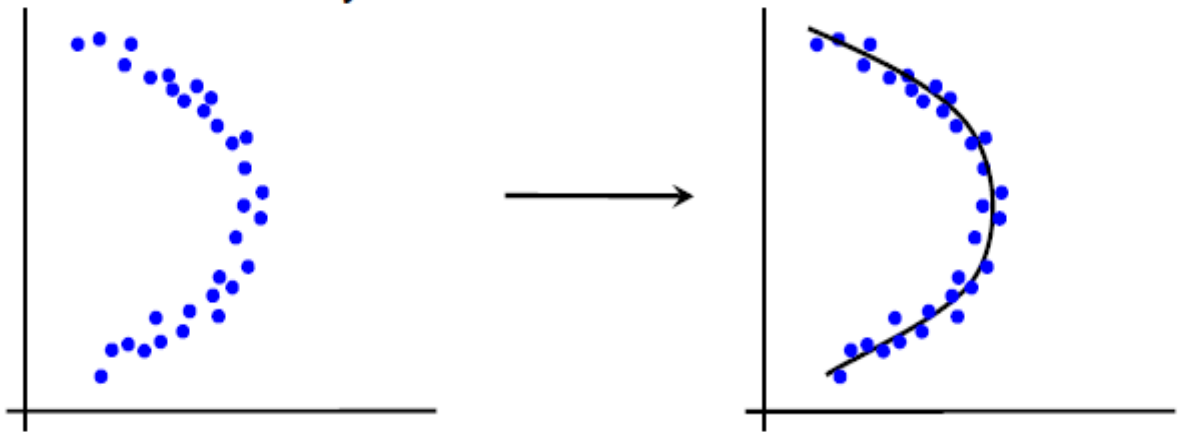


3. Unsupervised learning – model the data

- clustering

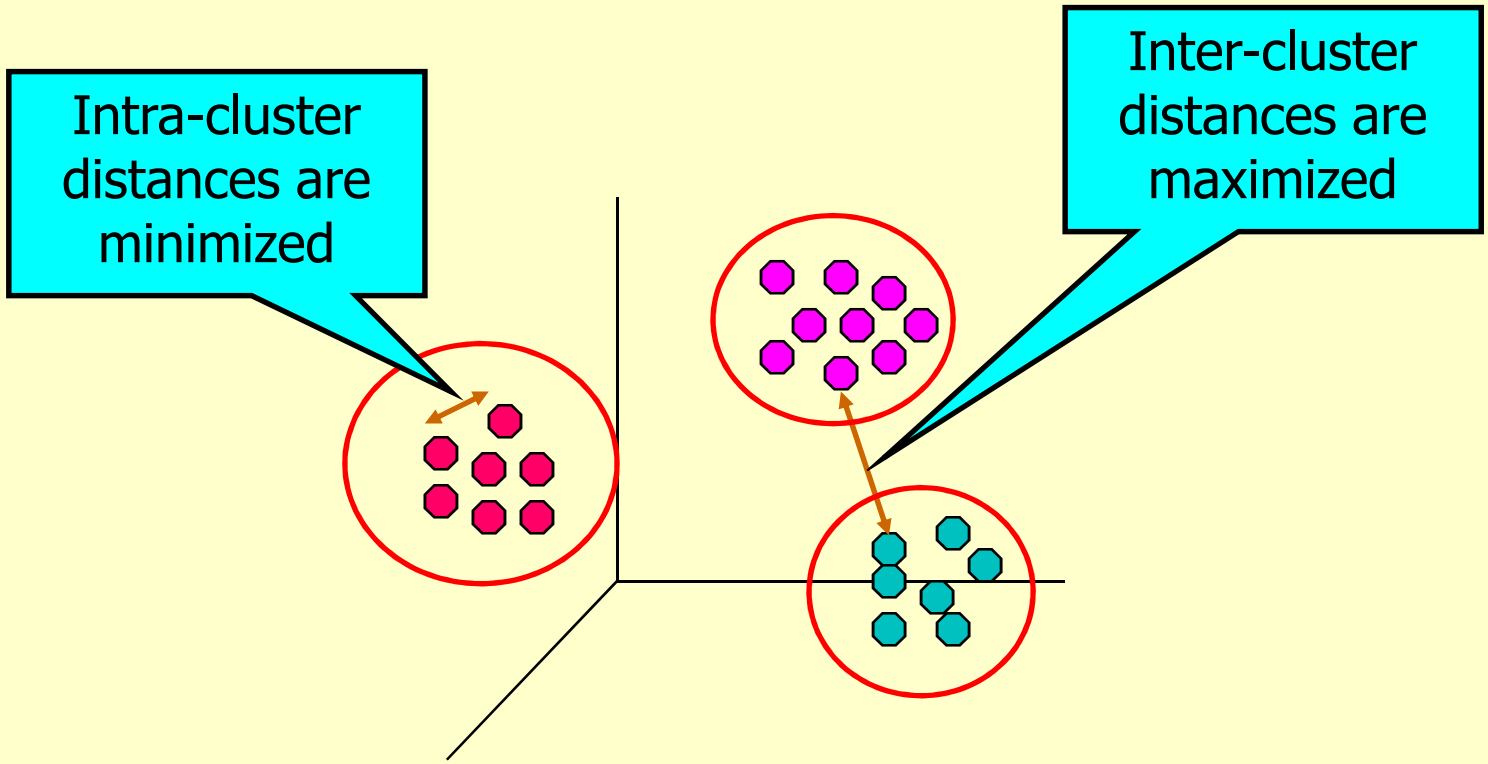


- dimensionality reduction



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

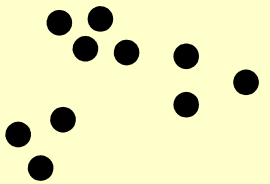


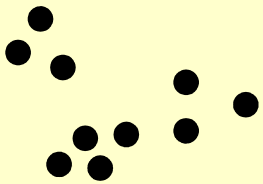
Clustering

- However,
  - Similarity is hard to define, and …. “We know it when we see it”
  - The real meaning of similarity is a philosophical question. We will take a more pragmatic approach.

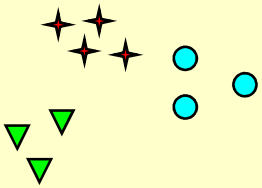
PC: http://www.funnyphotos.net.au/dog-owners/

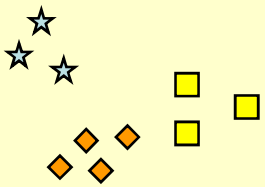
Notion of a Cluster can be Ambiguous



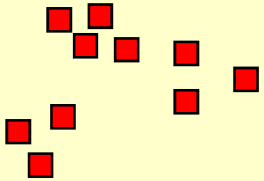


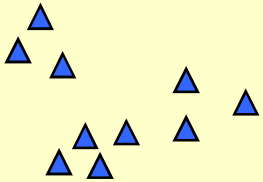
How many clusters?



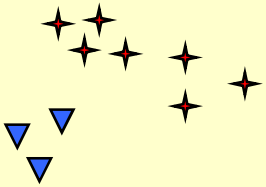


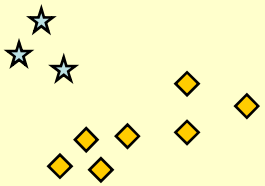
Six Clusters





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

Other Distinctions Between Sets of Clusters

- Exclusive versus non-exclusive
  - In non-exclusive clustering, 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 (membership) between 0 and 1
  - Weights must sum to 1
  - Each cluster is a fuzzy set.
- 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

K-MEANS CLUSTERING

- The **k-means algorithm** is an algorithm to cluster *n* objects based on attributes into *k* partitions, where $k < n$.
- It is similar to the expectation-maximization algorithm for mixtures of Gaussians in that they both attempt to find the centers of natural clusters in the data.
- It assumes that the object attributes form a vector space.

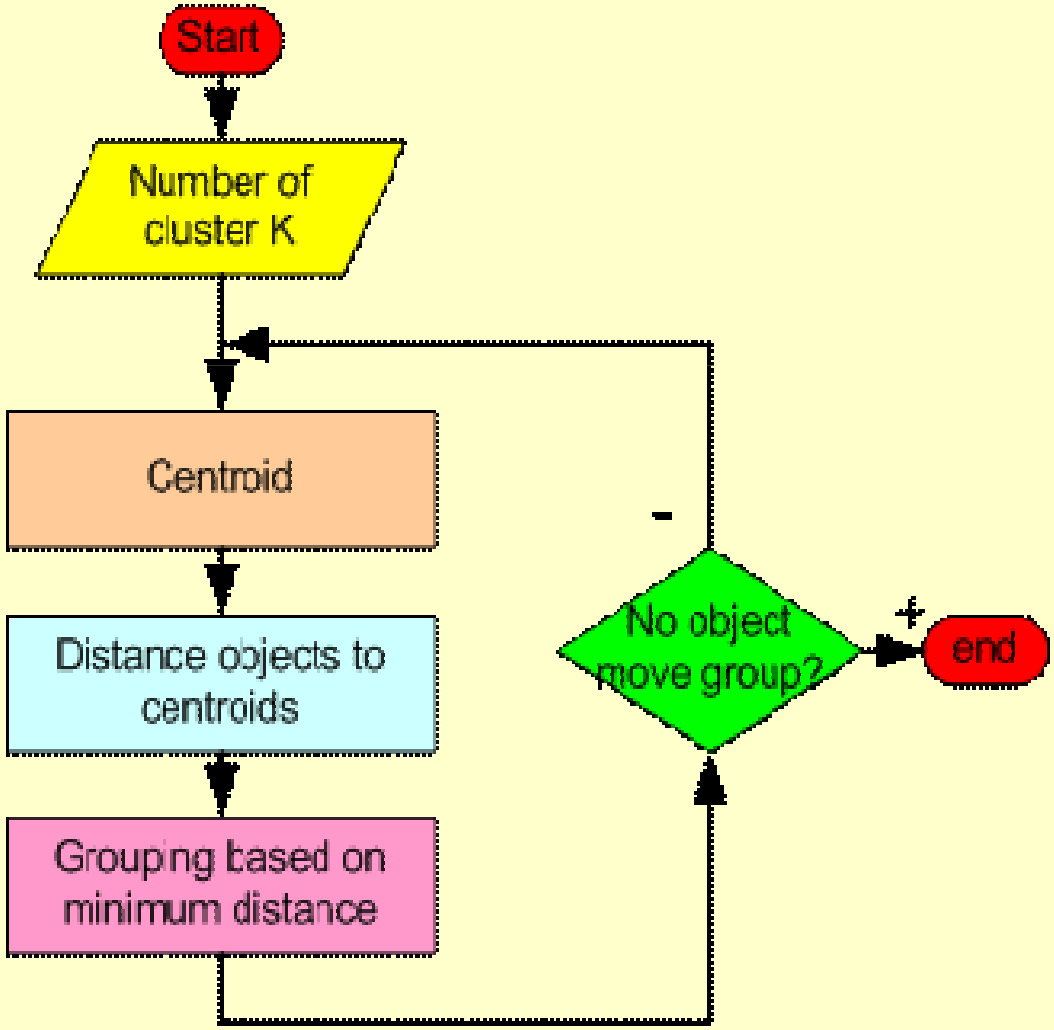
- An algorithm for partitioning (or clustering) *N* data points into *k* disjoint subsets S_j containing data points so as to minimize the sum-of-squares criterion

$$SSE = ICS(C_1, C_2, ..., C_k) = \sum_{j=1}^{k} \sum_{\vec{Z}_i \in C_i} d^2(\vec{Z}_i, \vec{V}_j)$$

  - Z_i is a data point in cluster C_j and V_j is the representative point (most often the mean) for cluster C_j .
  - 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 higher SSE than a poor clustering with higher k

- Simply speaking k-means clustering is an algorithm to classify or to group the objects based on attributes/features into K number of group.
- K is positive integer number.
- The grouping is done by minimizing the sum of squares of distances between data and the corresponding cluster centroid.

How the K-Mean Clustering algorithm works?



- **Step 1:** Begin with a decision on the value of k = number of clusters .
- **Step 2**: Put any initial partition that classifies the data into k clusters. You may assign the training samples randomly,or systematically as the following:

  1. Take the first k training sample as single-element clusters
  2. Assign each of the remaining (N-k) training sample to the cluster with the nearest centroid. After each assignment, recompute the centroid of the gaining cluster.

- **Step 3:** Take each sample in sequence and compute its distance from the centroid of each of the clusters. If a sample is not currently in the cluster with the closest centroid, switch this sample to that cluster and update the centroid of the cluster gaining the new sample and the cluster losing the sample.
- **Step 4 .** Repeat step 3 until convergence is achieved, that is until a pass through the training sample causes no new assignments.

A Simple example showing the implementation of *k*-means algorithm (using *k*=2)

Individual	Variable 1	Variable 2
1	1.0	1.0
2	1.5	2.0
3	3.0	4.0
4	5.0	7.0
5	3.5	5.0
6	4.5	5.0
7	3.5	4.5

Step 1:

Initialization: Randomly we choose following two centroids (k=2) for two clusters.

In this case the 2 centroid are: m1=(1.0,1.0) and m2=(5.0,7.0).

Individual	Variable 1	Variable 2
1	1.0	1.0
2	1.5	2.0
3	3.0	4.0
4	5.0	7.0
5	3.5	5.0
6	4.5	5.0
7	3.5	4.5

	Individual	Mean Vector
Group 1	1	(1.0, 1.0)
Group 2	4	(5.0, 7.0)

Step 2:

- Thus, we obtain two clusters containing:

  {1,2,3} and {4,5,6,7}.
- Their new centroids are:

Individual	Centroid 1	Centroid 2
1	0	7.21
2 (1.5, 2.0)	1.12	6.10
3	3.61	3.61
4	7.21	0
5	4.72	2.5
6	5.31	2.06
7	4.30	2.92

$$m_1 = \left(\frac{1}{3}(1.0+1.5+3.0), \frac{1}{3}(1.0+2.0+4.0)\right) = (1.83, 2.33)$$

$$m_2 = \left(\frac{1}{4}(5.0+3.5+4.5+3.5), \frac{1}{4}(7.0+5.0+5.0+4.5)\right)$$

$$= (4.12, 5.38)$$

$$d(m_1, 2) = \sqrt{|1.0-1.5|^2 + |1.0-2.0|^2} = 1.12$$

$$d(m_2, 2) = \sqrt{|5.0-1.5|^2 + |7.0-2.0|^2} = 6.10$$

Step 3:

- Now using these centroids we compute the Euclidean distance of each object, as shown in table.

- Therefore, the new clusters are:

  {1,2} and {**3**,4,5,6,7}

- Next centroids are: m1=(1.25,1.5) and m2 = (3.9,5.1)

Individual	Centroid 1	Centroid 2
1	1.57	5.38
2	0.47	4.28
3	2.04	1.78
4	5.64	1.84
5	3.15	0.73
6	3.78	0.54
7	2.74	1.08

- Step 4 :

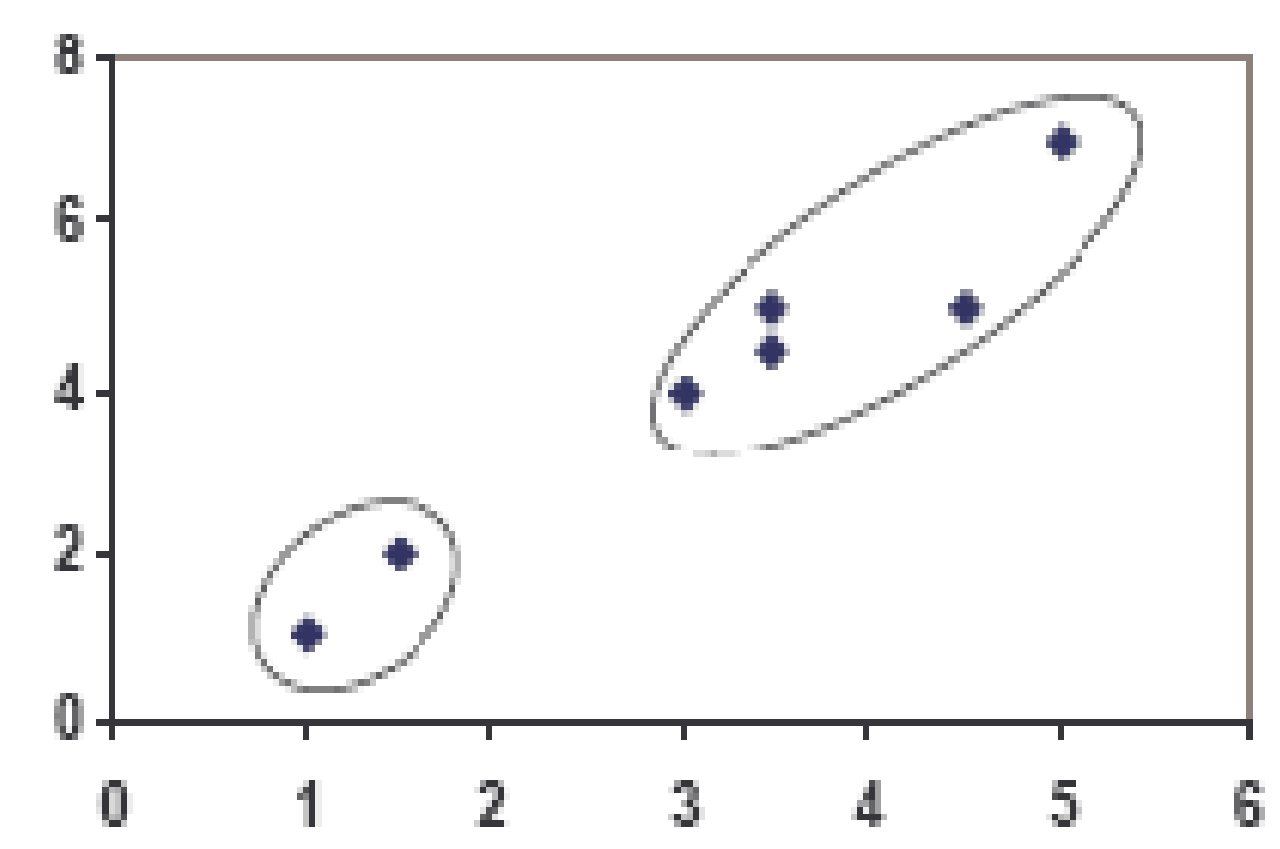
  The clusters obtained are:

  {1,2} and {3,4,5,6,7}

- Therefore, there is no change in the cluster.
- Thus, the algorithm comes to a halt here and final result consist of 2 clusters {1,2} and {3,4,5,6,7}.

Individual	Centroid 1	Centroid 2
1	0.56	5.02
2	0. 56	3.92
3	3.05	1.42
4	6.66	2.20
5	4.16	0.41
6	4.78	0.61
7	3.75	0.72

PLOT



(with K=3)

Individual	$m_1 = 1$	$m_2 = 2$	$m_3 = 3$	cluster
1	0	1.11	3.61	1
2	1.12	0	2.5	2
3	3.61	2.5	0	3
4	7.21	6.10	3.61	3
5	4.72	3.61	1.12	3
6	5.31	4.24	1.80	3
7	4.30	3.20	0.71	3

C_3

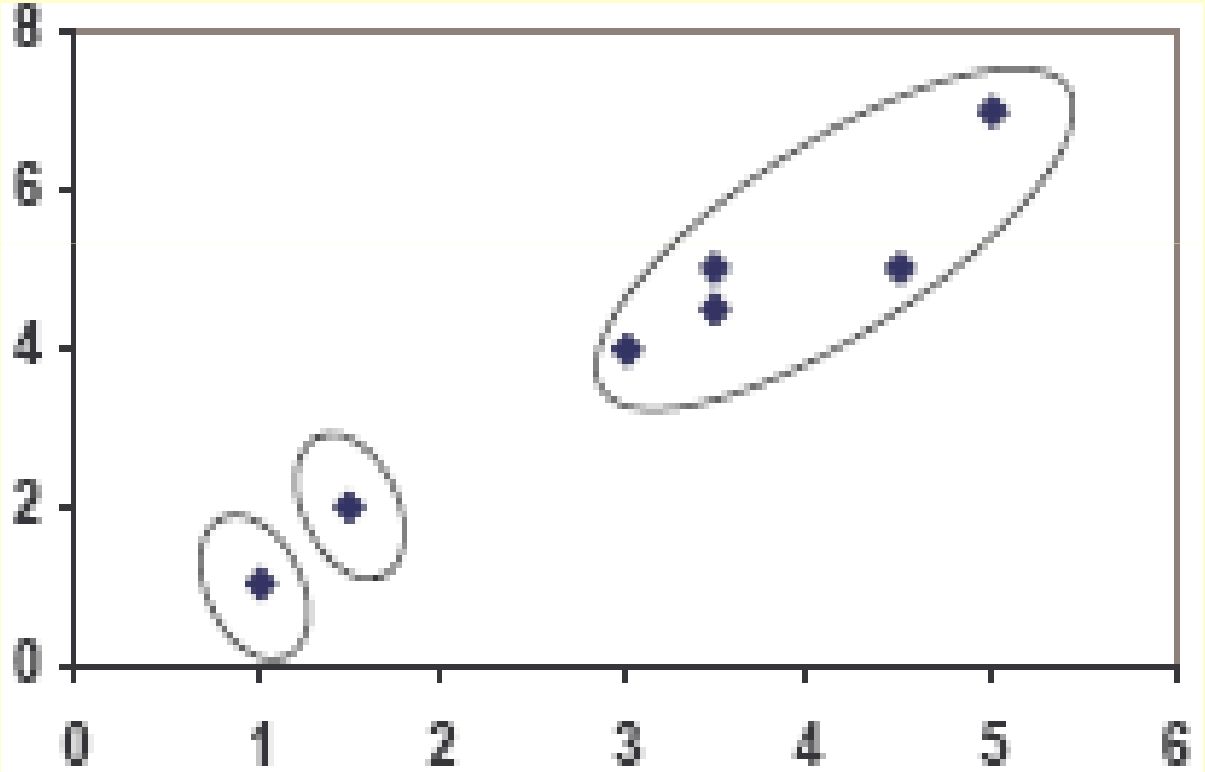
clustering with initial centroids (1, 2, 3)

Step 1

Individual	m_1 (1.0, 1.0)	m_2 (1.5, 2.0)	m_3 (3.9,5.1)	cluster
1	0	1.11	5.02	1
2	1.12	0	3.92	2
3	3.61	2.5	1.42	3
4	7.21	6.10	2.20	3
5	4.72	3.61	0.41	3
6	5.31	4.24	0.61	3
7	4.30	3.20	0.72	3

Step 2

PLOT



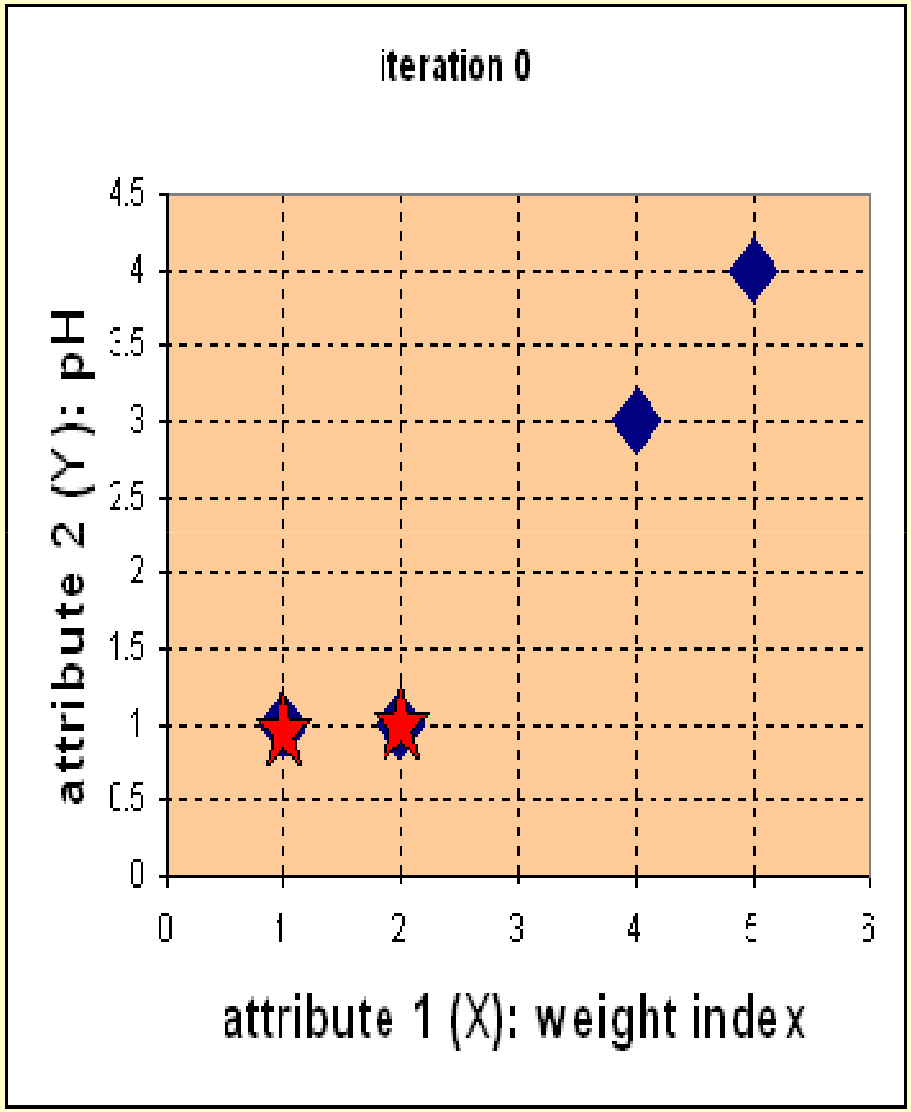
Real-Life Numerical Example of K-Means Clustering

We have 4 medicines as our training data points object and each medicine has 2 attributes. Each attribute represents coordinate of the object. We have to determine which medicines belong to cluster 1 and which medicines belong to the other cluster.

Object	Attribute1 (X): weight index	Attribute 2 (Y): pH
Medicine A	1	1
Medicine B	2	1
Medicine C	4	3
Medicine D	5	4

Step 1:

- **Initial value of centroids** : Suppose we use medicine A and medicine B as the first centroids.
- Let and c_1 and c_2 denote the coordinate of the centroids, then $c_1=(1,1)$ and $c_2=(2,1)$



- **Objects-Centroids distance** : we calculate the distance between cluster centroid to each object. Let us use Euclidean distance, then we have distance matrix at iteration 0 is

$$\mathbf{D}^0 = \begin{bmatrix} 0 & 1 & 3.61 & 5 \\ 1 & 0 & 2.83 & 4.24 \end{bmatrix} \quad \begin{matrix} \mathbf{c}_1 = (1,1) & group-1 \\ \mathbf{c}_2 = (2,1) & group-2 \end{matrix}$$

$$\begin{matrix} A & B & C & D \end{matrix}$$

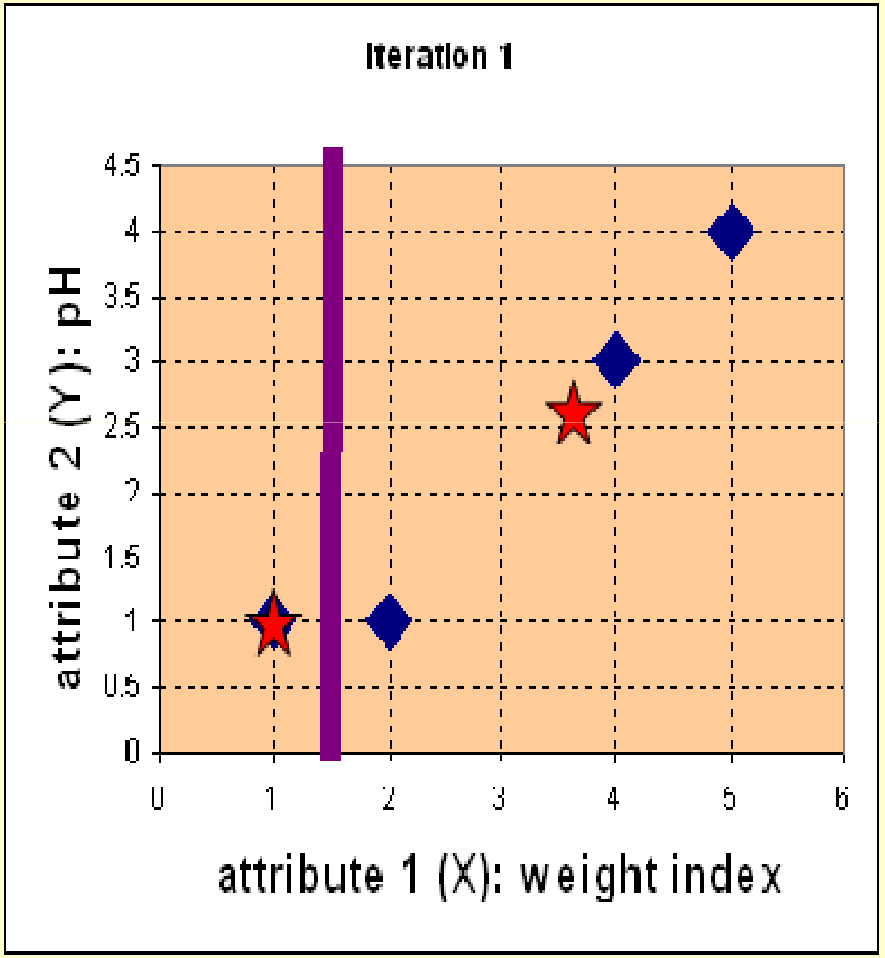
$$\begin{bmatrix} 1 & 2 & 4 & 5 \\ 1 & 1 & 3 & 4 \end{bmatrix} \quad \begin{matrix} X \\ Y \end{matrix}$$

- Each column in the distance matrix symbolizes the object.
- The first row of the distance matrix corresponds to the distance of each object to the first centroid and the second row is the distance of each object to the second centroid.
- For example, distance from medicine C = (4, 3) to the first centroid $\mathbf{c}_1 = (1,1)$ is , $\sqrt{(4-1)^2+(3-1)^2} = 3.61$ and its distance to the second centroid is , $\mathbf{c}_2 = (2,1)$ is $\sqrt{(4-2)^2+(3-1)^2} = 2.83$ etc.

Step 2:

- **Objects clustering** : We assign each object based on the minimum distance.
- Medicine A is assigned to group 1, medicine B to group 2, medicine C to group 2 and medicine D to group 2.
- The elements of Group matrix below is 1 if and only if the object is assigned to that group.

$$G^0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \end{bmatrix} \begin{matrix} group-1 \\ group-2 \end{matrix}$$
$$A \quad B \quad C \quad D$$



- **<u>Iteration-1, Objects-Centroids distances</u>** : The next step is to compute the distance of all objects to the new centroids.
- Similar to step 2, we have distance matrix at iteration 1 is

$$D^1 = \begin{bmatrix} 0 & 1 & 3.61 & 5 \\ 3.14 & 2.36 & 0.47 & 1.89 \end{bmatrix} \quad \begin{matrix} c_1 = (1,1) & group-1 \\ c_2 = (\frac{11}{3}, \frac{8}{3}) & group-2 \end{matrix}$$

$$\begin{matrix} A & B & C & D \end{matrix}$$

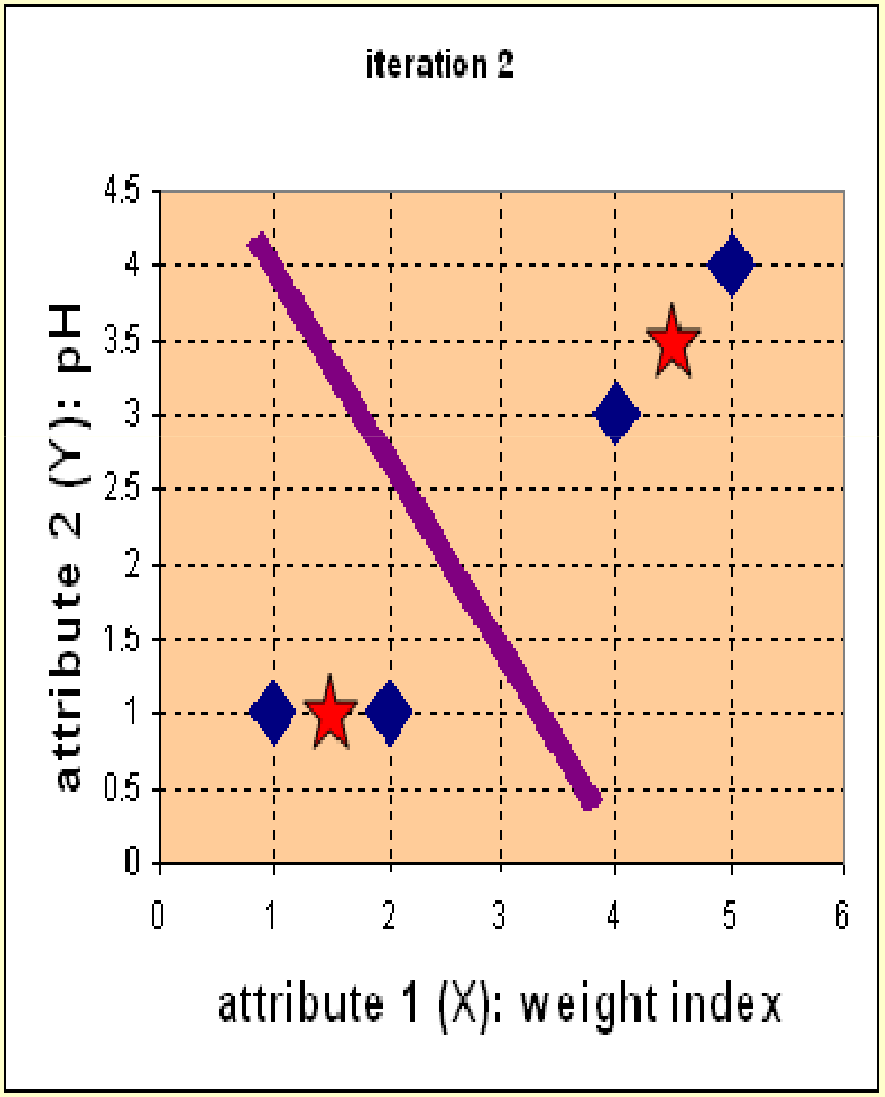
$$\begin{bmatrix} 1 & 2 & 4 & 5 \\ 1 & 1 & 3 & 4 \end{bmatrix} \quad \begin{matrix} X \\ Y \end{matrix}$$

- **Iteration-1, Objects clustering:** Based on the new distance matrix, we move the medicine B to Group 1 while all the other objects remain. The Group matrix is shown below

$$G^1 = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix} \quad \begin{matrix} group-1 \\ group-2 \end{matrix}$$

$$A \quad B \quad C \quad D$$

- **Iteration 2, determine centroids:** Now we repeat step 4 to calculate the new centroids coordinate based on the clustering of previous iteration. Group1 and group 2 both has two members, thus the new centroids are $c_1 = (\frac{1+2}{2}, \frac{1+1}{2}) = (1\frac{1}{2}, 1)$ and $c_2 = (\frac{4+5}{2}, \frac{3+4}{2}) = (4\frac{1}{2}, 3\frac{1}{2})$



- **<u>Iteration-2, Objects-Centroids distances</u>**
  : Repeat step 2 again, we have new distance matrix at iteration 2 as

$$\mathbf{D}^2 = \begin{bmatrix} 0.5 & 0.5 & 3.20 & 4.61 \\ 4.30 & 3.54 & 0.71 & 0.71 \end{bmatrix} \quad \begin{matrix} \mathbf{c}_1 = (1\frac{1}{2}, 1) \quad group-1 \\ \mathbf{c}_2 = (4\frac{1}{2}, 3\frac{1}{2}) \quad group-2 \end{matrix}$$

$$\begin{matrix} A & B & C & D \end{matrix}$$

$$\begin{bmatrix} 1 & 2 & 4 & 5 \\ 1 & 1 & 3 & 4 \end{bmatrix} \begin{matrix} X \\ Y \end{matrix}$$

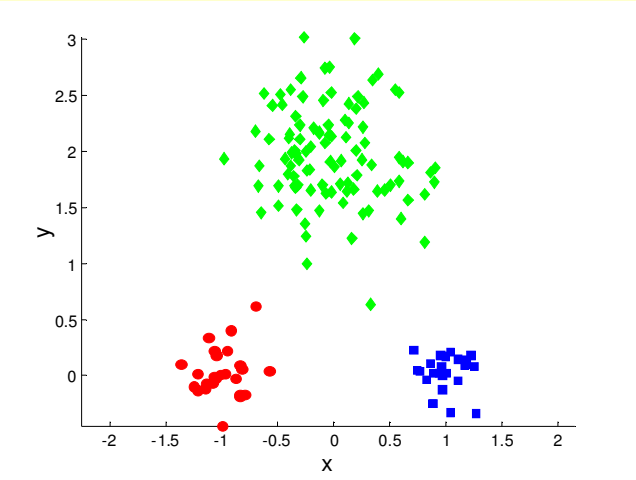
- **<u>Iteration-2, Objects clustering:</u>** Again, we assign each object based on the minimum distance.

$$\mathbf{G}^2 = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix} \begin{matrix} group-1 \\ group-2 \end{matrix}$$

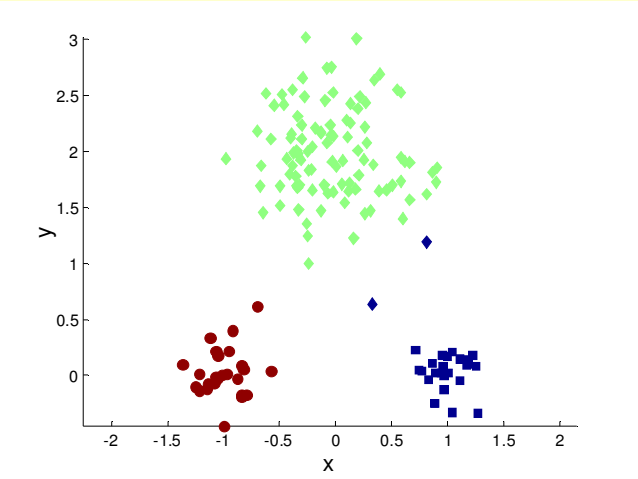
$$A \quad B \quad C \quad D$$

- We obtain result that $\mathbf{G}^2 = \mathbf{G}^1$. Comparing the grouping of last iteration and this iteration reveals that the objects does not move group anymore.
- Thus, the computation of the k-mean clustering has reached its stability and no more iteration is needed..

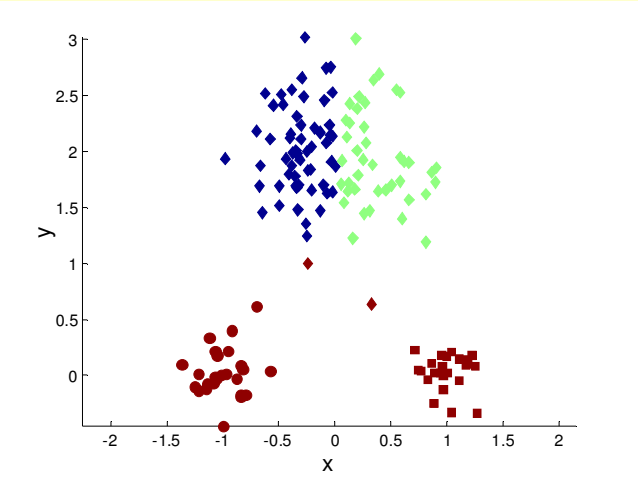
Two different K-means Clustering



Original Points

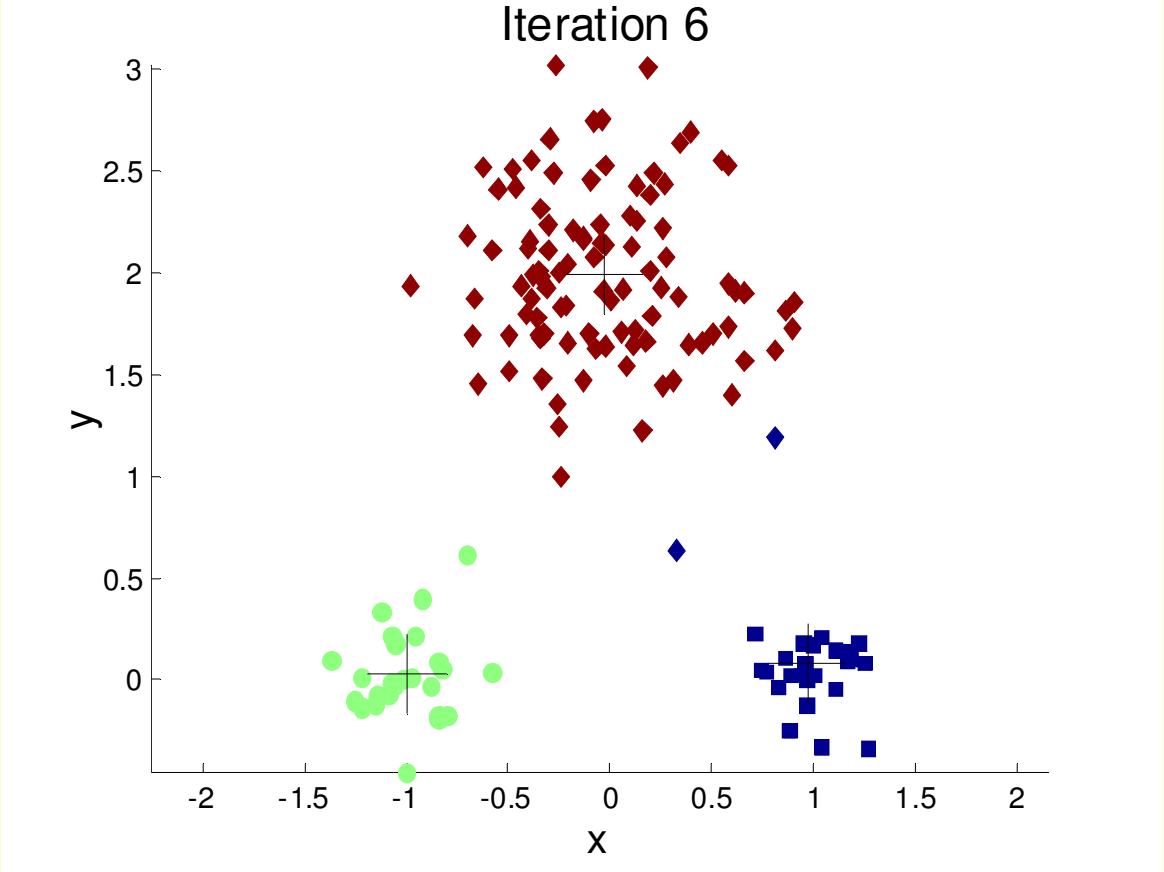


Optimal Clustering

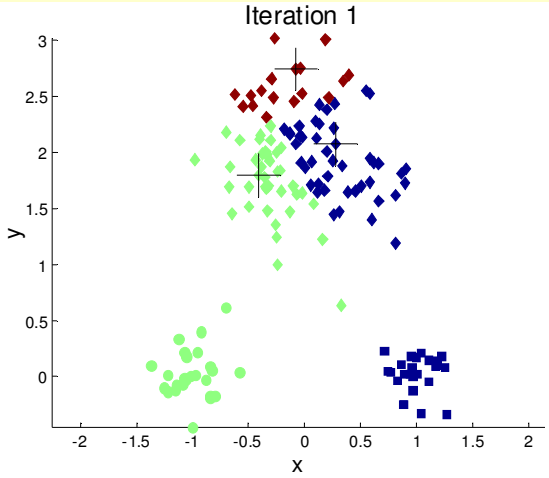


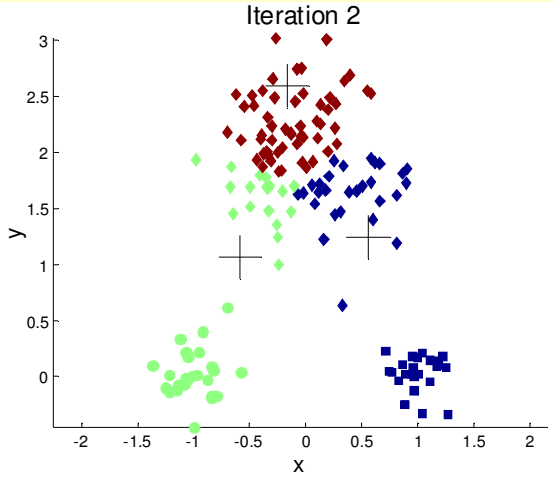
Sub-optimal Clustering

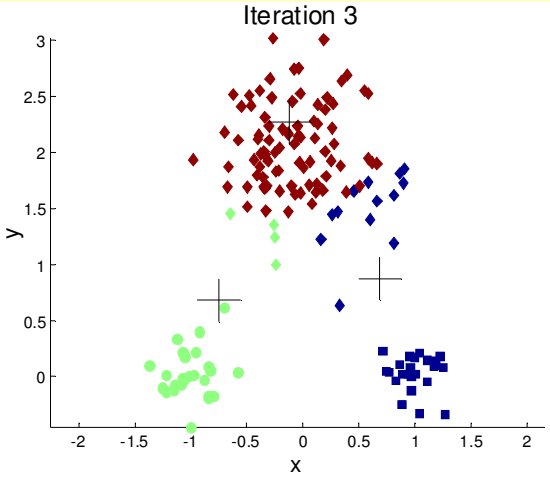
Importance of Choosing Initial Centroids

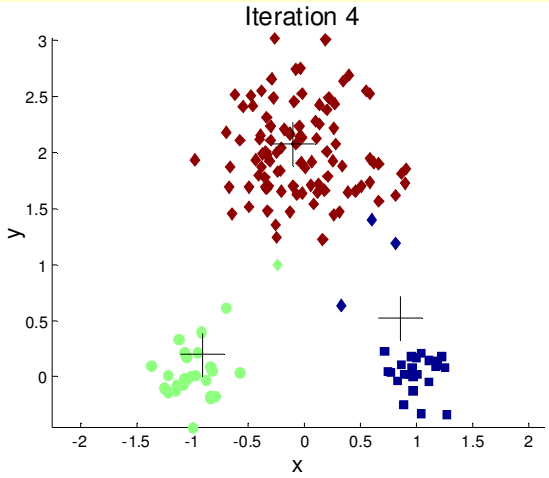


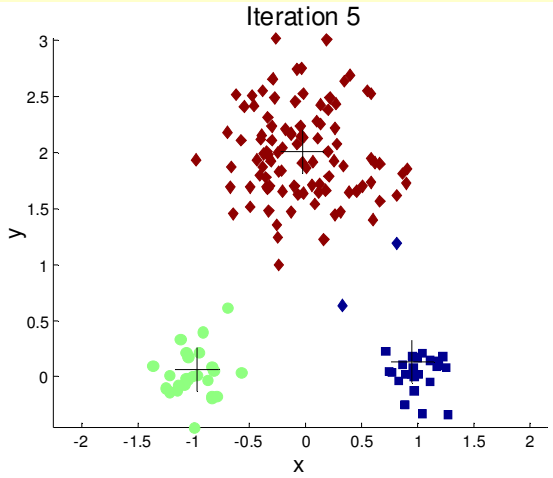
Importance of Choosing Initial Centroids

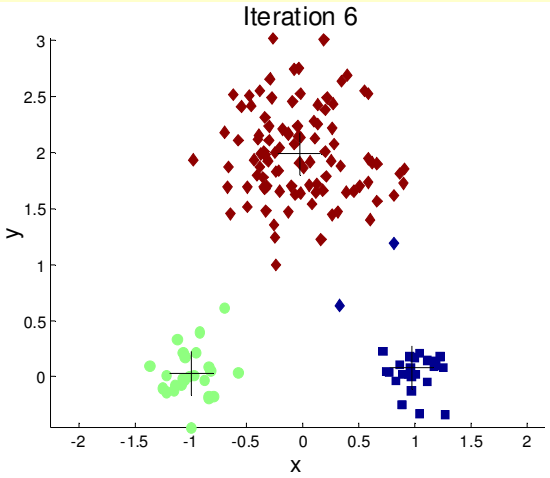




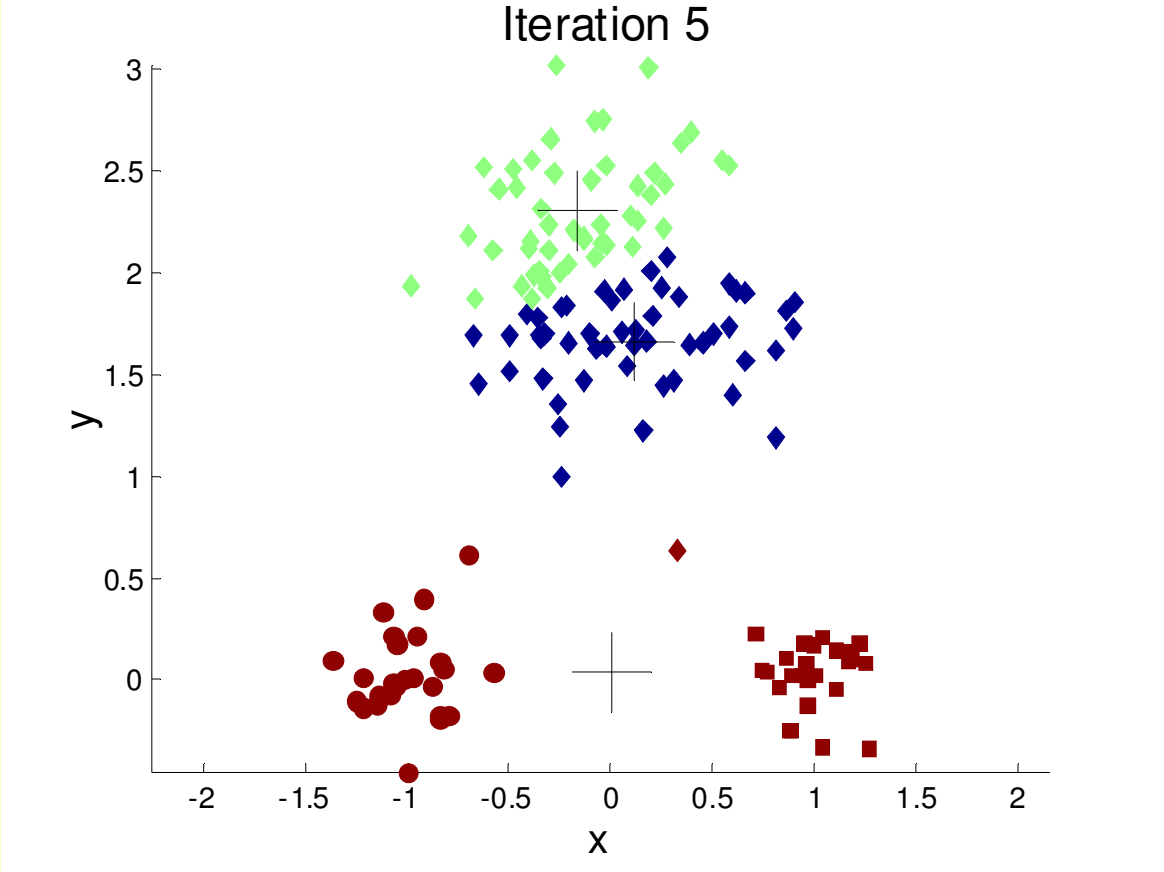








Importance of Choosing Initial Centroids …

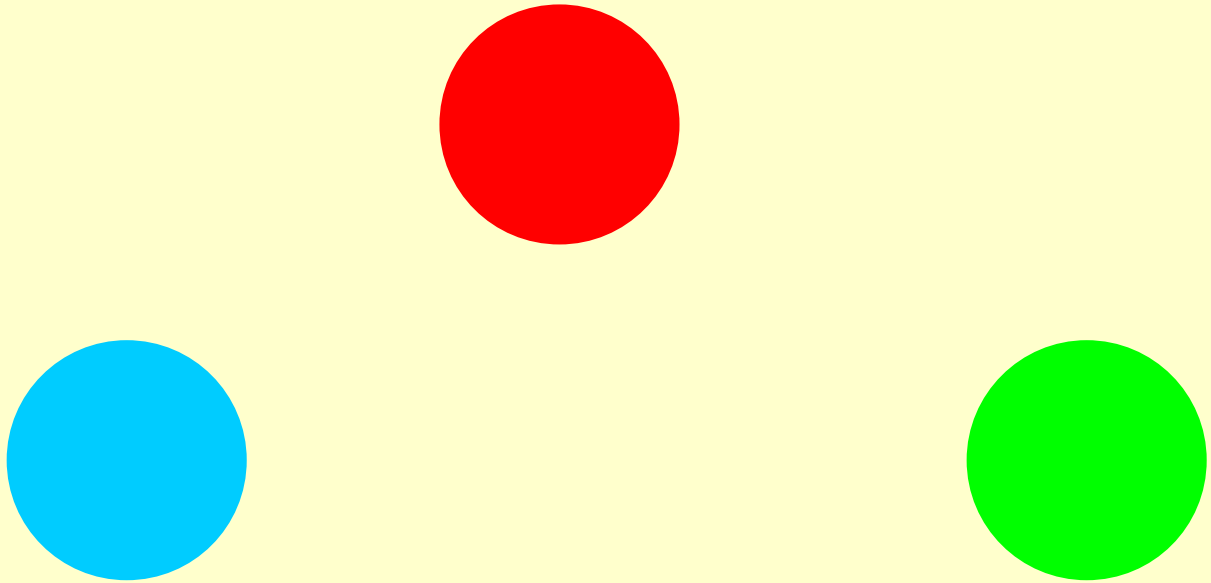


Types of Clusters

- Well-separated clusters
- Center-based clusters
- Contiguous clusters
- Density-based clusters
- Property or Conceptual
- Described by an Objective Function

Types of Clusters: Well-Separated

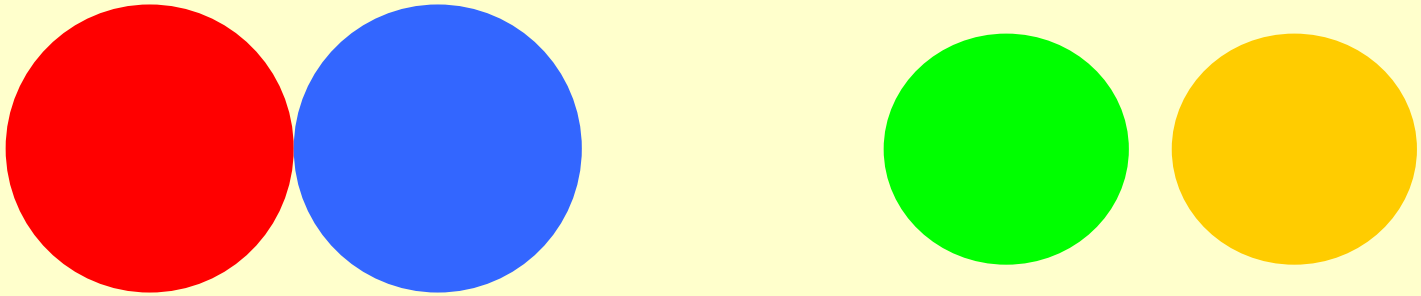
- Well-Separated Clusters:
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.



3 well-separated clusters

Types of Clusters: Center-Based

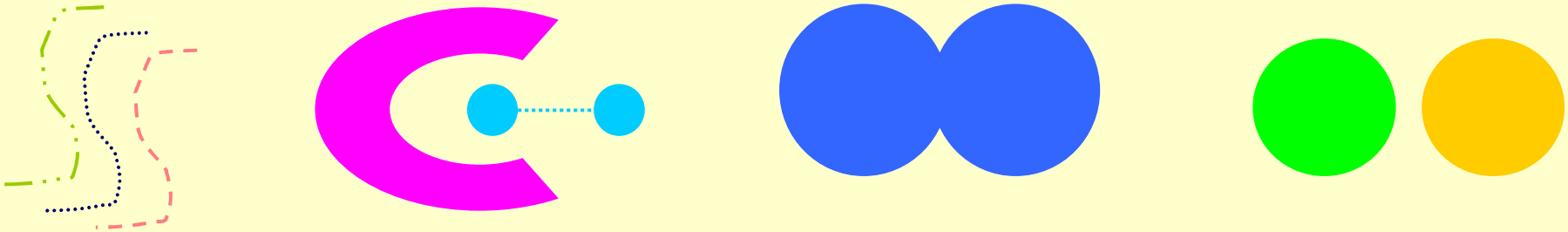
- Center-based
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the “center” of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the average of all the points in the cluster, or a medoid, the most “representative”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



4 center-based clusters

Types of Clusters: Contiguity-Based

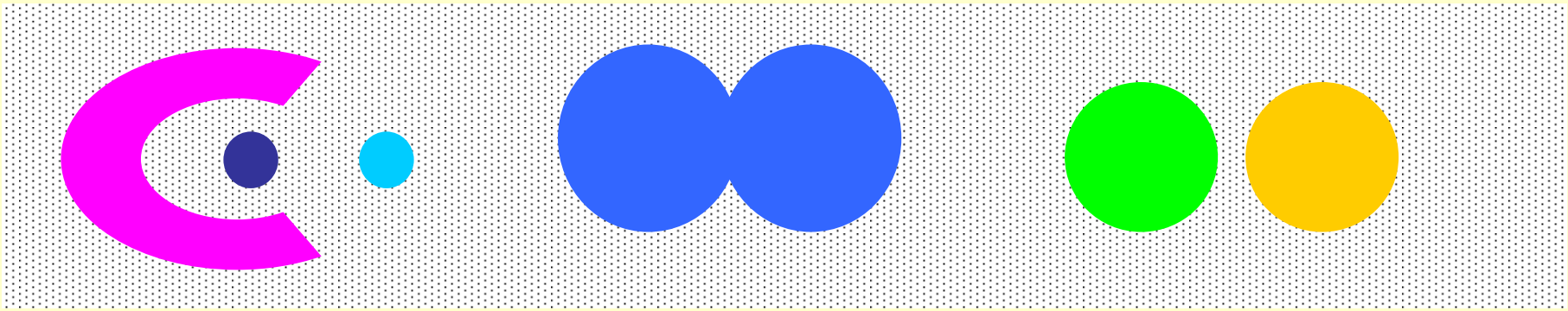
- Contiguous Cluster (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.



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.

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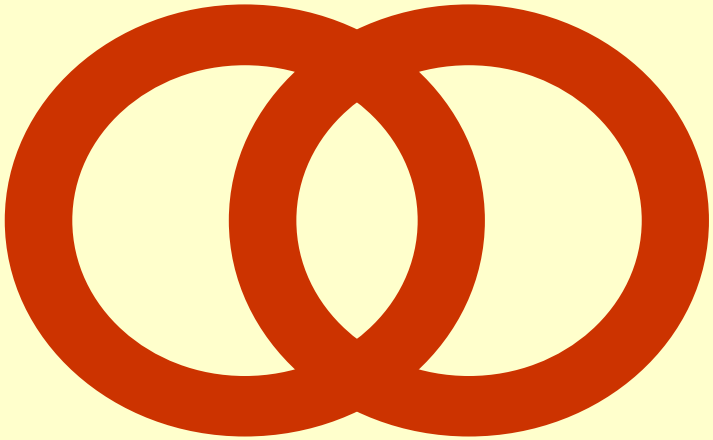


2 Overlapping Circles

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. (No. of feasible partitions could be very large and the problem is 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

Evaluating K-means Clusters

- Most common measure is Sum of Squared Error (SSE) or summed Intra Cluster Spread (ICS)
  - For each point, the error is the distance to the nearest cluster center
  - To get SSE, we square these errors and sum them.

$$SSE = ICS(C_1, C_2, ..., C_k) = \sum_{j=1}^{k} \sum_{\vec{Z}_i \in C_i} d^2(\vec{Z}_i, \vec{m}_j)$$

  - Z_j is a data point in cluster C_i and m_j is the representative point for cluster C_i
    - can show that m_j 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

skip

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

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

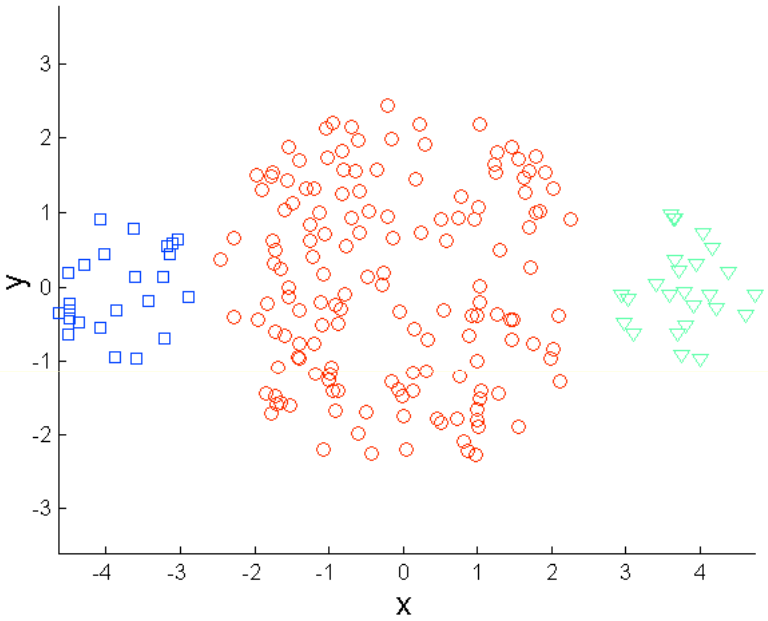
- Several strategies
  - Choose the point that contributes most to SSE
  - Choose a point from the cluster with the highest SSE
  - If there are several empty clusters, the above can be repeated several times.

Limitations of K-means

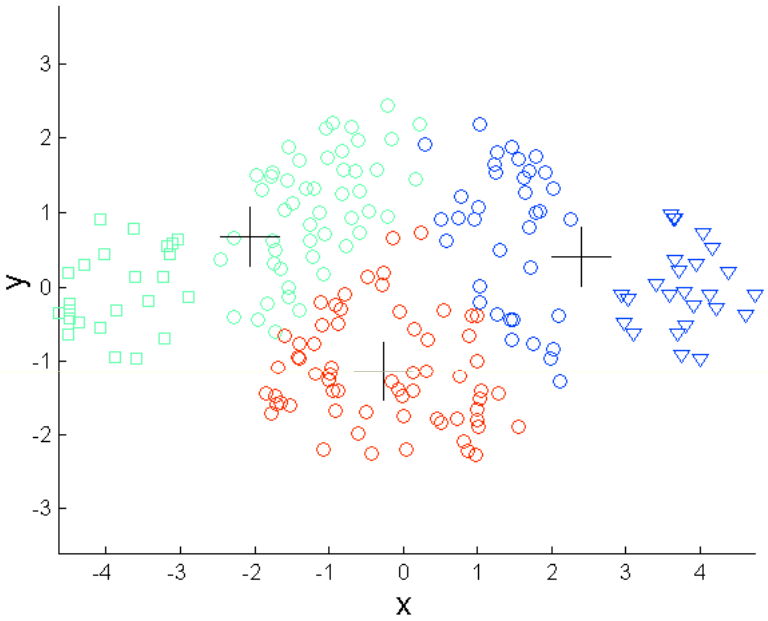
- K-means has problems when clusters are of differing
  - Sizes
  - Densities
  - Non-globular shapes

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

Limitations of K-means: Differing Sizes

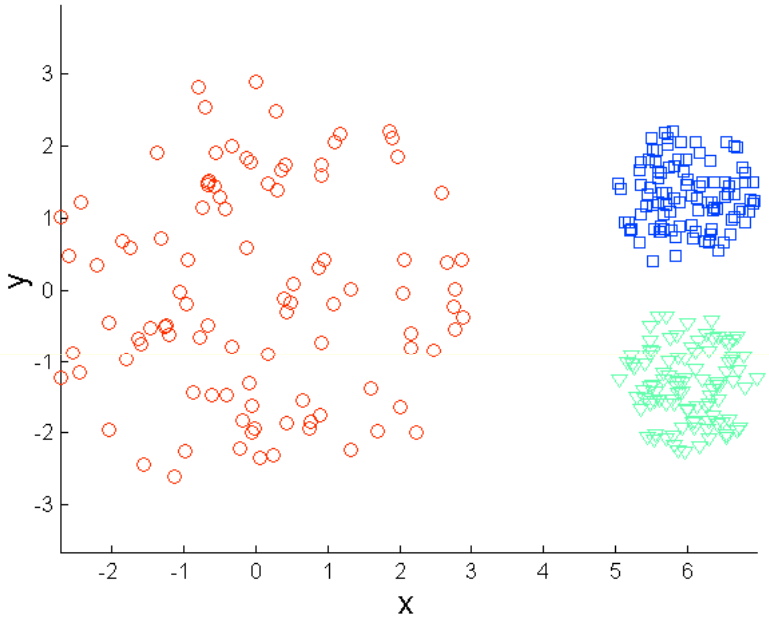


Original Points

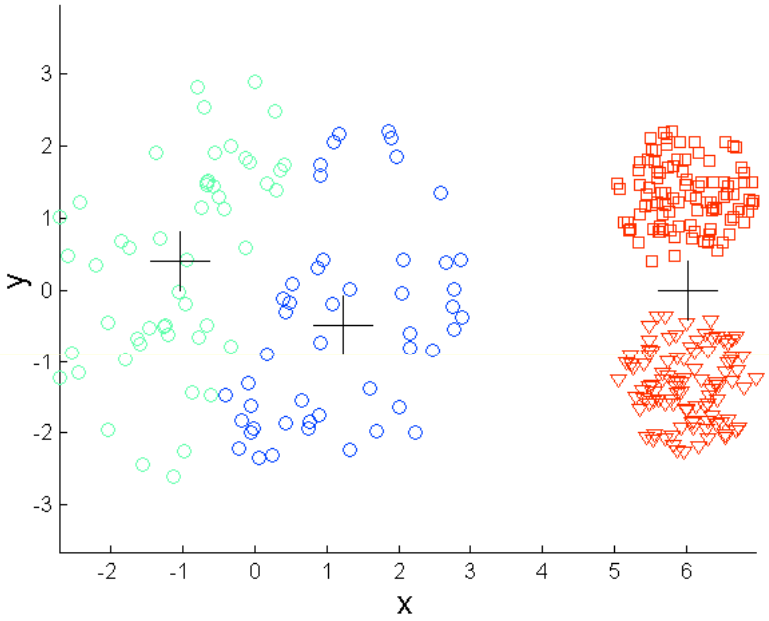


K-means (3 Clusters)

Limitations of K-means: Differing Density

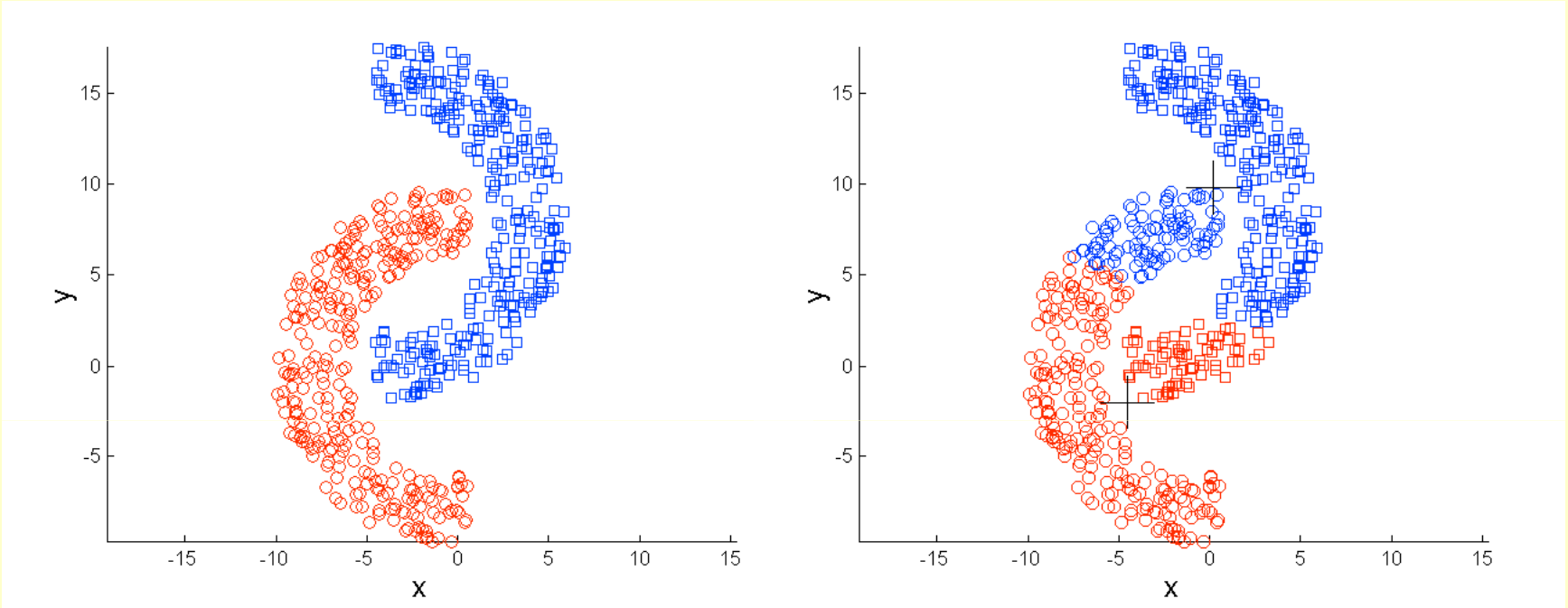


Original Points



K-means (3 Clusters)

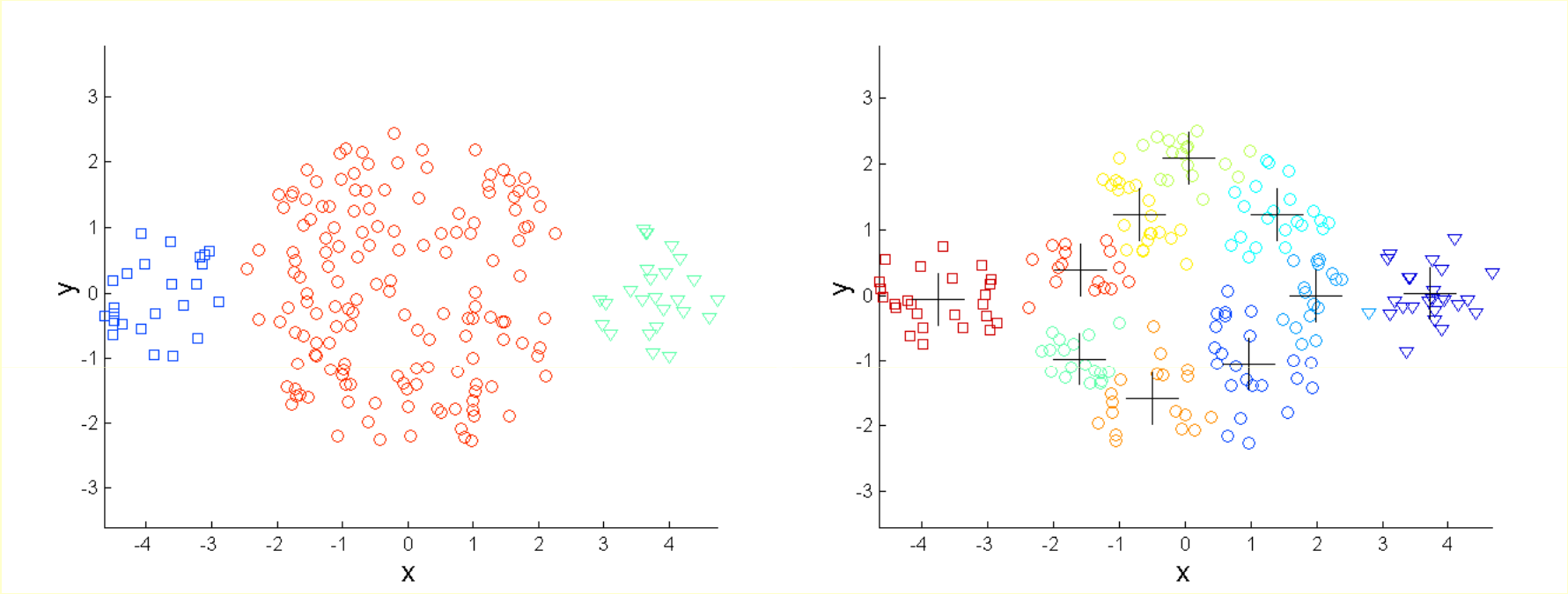
Limitations of K-means: Non-globular and linearly non-separable Shapes



Original Points

K-means (2 Clusters)

Overcoming K-means Limitations



Original Points **K-means Clusters**

One solution is to use many clusters.

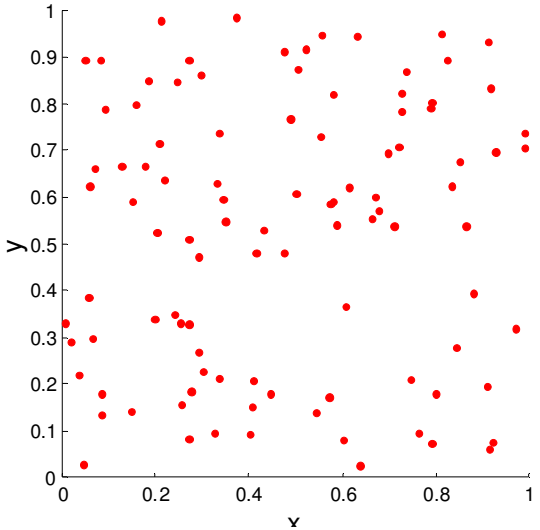
Find parts of clusters, but need to put together.

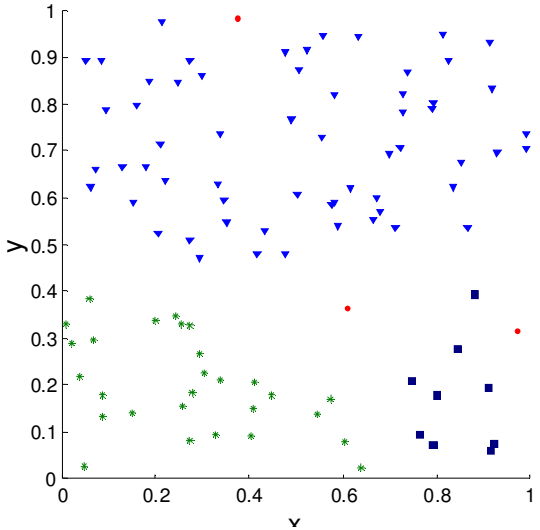
Cluster Validity

- 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”!
- 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

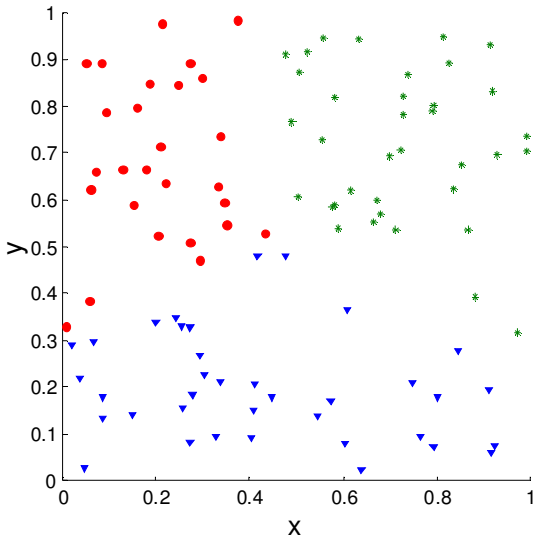
Random Points

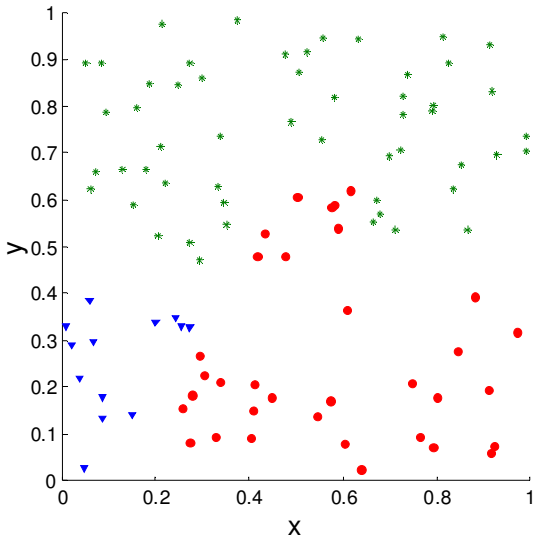




DBSCAN

K-means





Complete Link

Different Aspects of Cluster Validation

1. Determining the clustering tendency of a set of data, i.e., distinguishing whether non-random structure actually exists in the data.
2. Comparing the results of a cluster analysis to externally known results, e.g., to externally given class labels.
3. Evaluating how well the results of a cluster analysis fit the data *without* reference to external information.
    - Use only the data
4. Comparing the results of two different sets of cluster analyses to determine which is better.
5. Determining the 'correct' number of clusters.

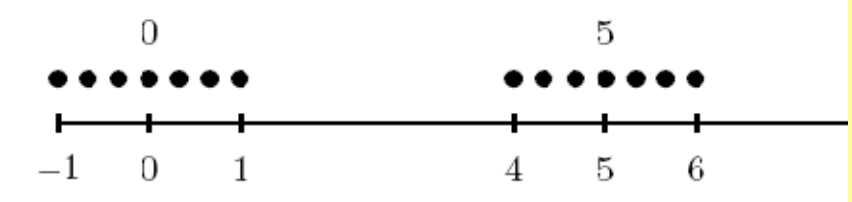
For 2, 3, and 4, we can further distinguish whether we want to evaluate the entire clustering or just individual clusters.

Landscape for Clustering Problem

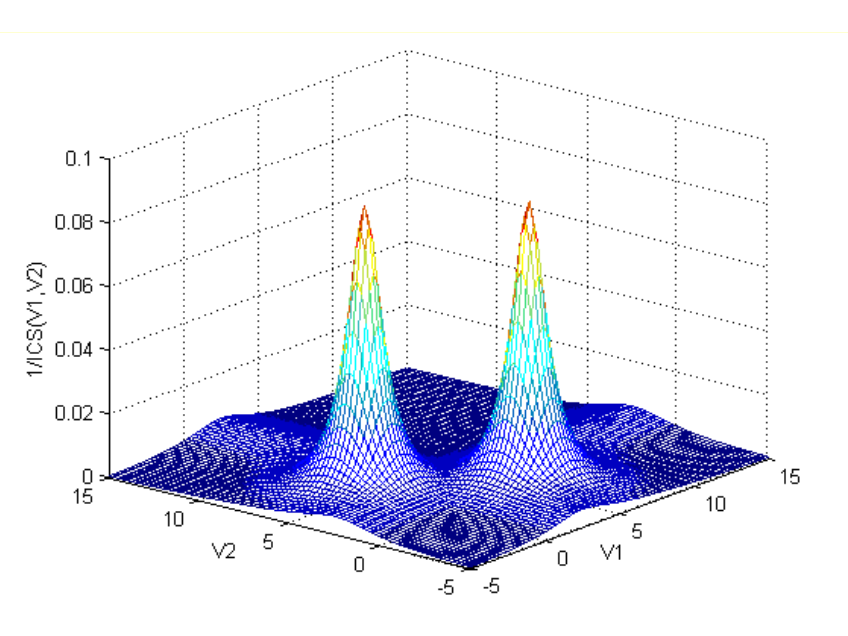
The k-means objective function

$$ICS(C_1, C_2, ..., C_k) = \sum_{j=1}^{k} \sum_{\vec{Z}_i \in C_i} d^2(\vec{Z}_i, \vec{m}_j)$$

Example of an extremely simple one-dimensional dataset

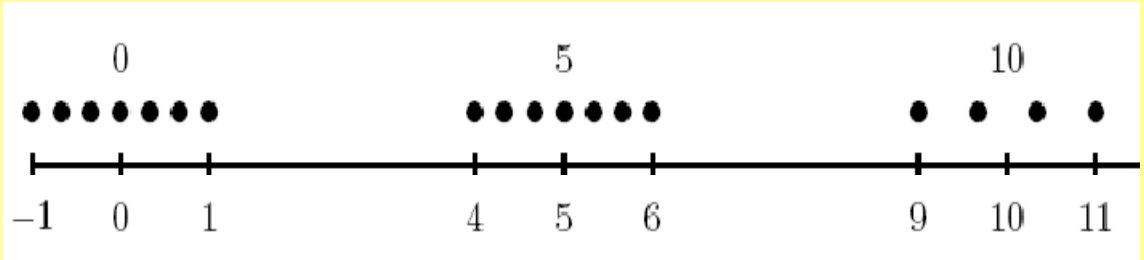


Fitness function (Reciprocal of ICS) plot of the hard c-means algorithm for above dataset

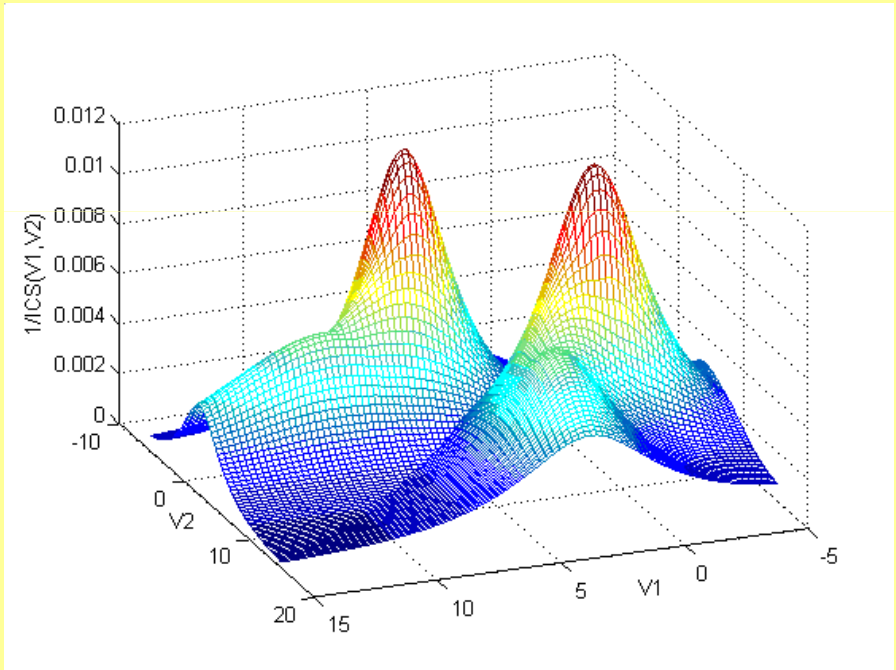


Landscape for Clustering Problem (Contd.)

The previous data but now
With some noise points



Fitness function (Reciprocal of ICS) plot of the hard c-means algorithm for above dataset



In addition to two global minima, we have local minima at: approximately (0, 10), (5, 10), (10, 0), (10, 5). For these local minima one prototype covers one of the data clusters, while the other prototype is mislead to the noise cluster.

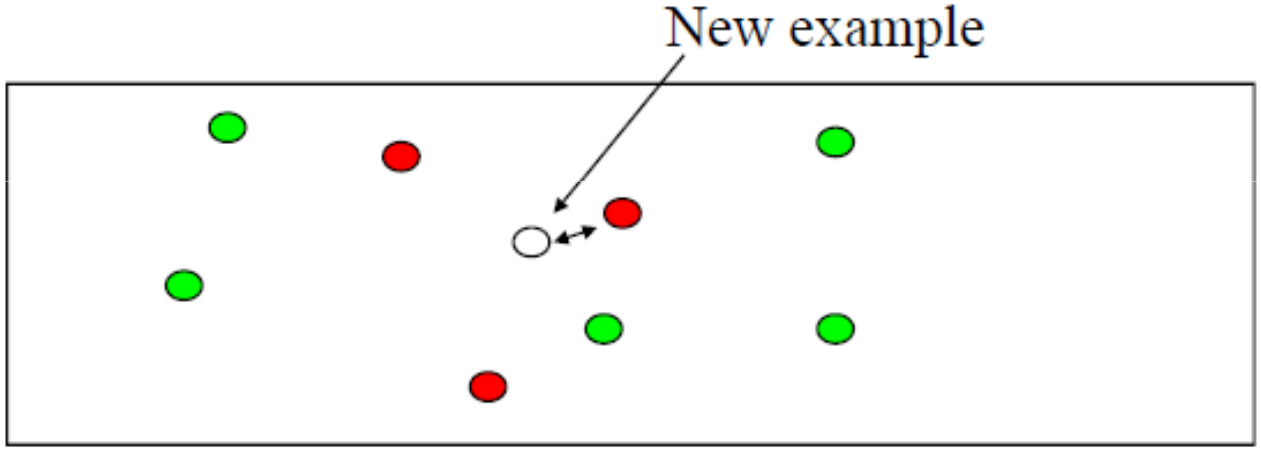
K Nearest Neighbor Classifiers

The Nearest Neighbor Algorithm

- A **lazy learning** algorithm
  - The "learning" does not occur until the test example is given
  - In contrast to so called "eager learning" algorithms (which carries out learning without knowing the test example, and after learning training examples can be discarded)

Nearest Neighbor Algorithm

- Remember all training examples
- Given a new example **x**, find the its closest training example <$\mathbf{x}^i$, y^i> and predict y^i

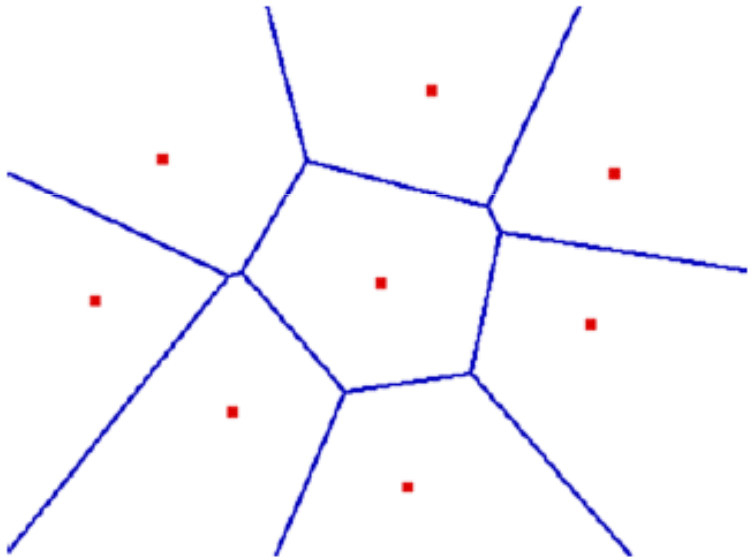


- How to measure distance – Euclidean (squared):

$$\left\|\mathbf{x}-\mathbf{x}^i\right\|^2=\sum_j(x_j-x_j^i)^2$$

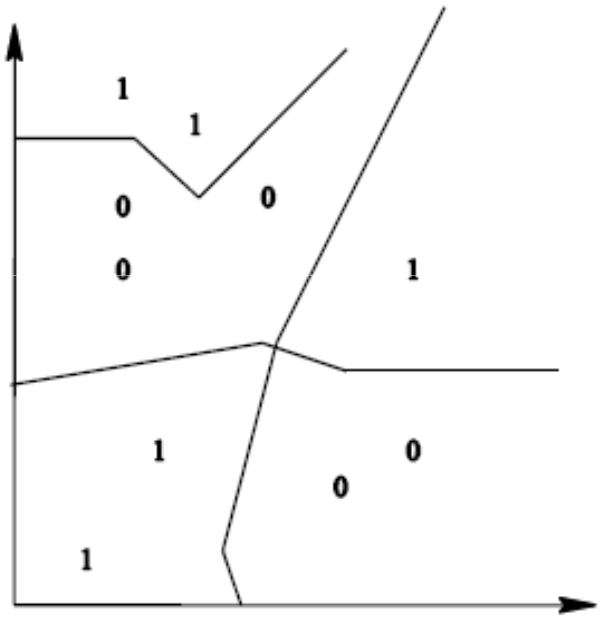
Decision Boundaries: The Voronoi Diagram

- Given a set of points, a **Voronoi diagram** describes the areas that are nearest to any given point.
- These areas can be viewed as zones of control.

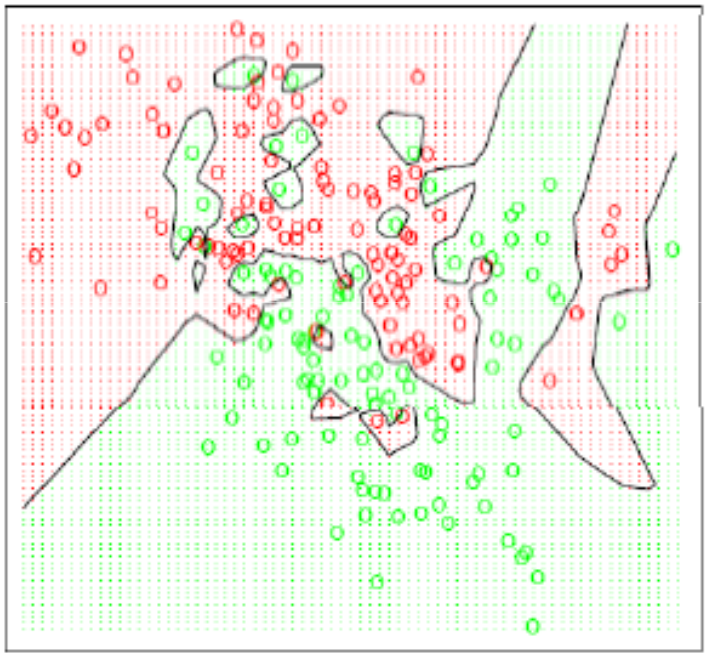


Decision Boundaries: The Voronoi Diagram

- Decision boundaries are formed by a **subset** of the Voronoi diagram of the training data
- Each line segment is equidistant between two points **of opposite class**.
- The more examples that are stored, the more fragmented and complex the decision boundaries can become.



Decision Boundaries

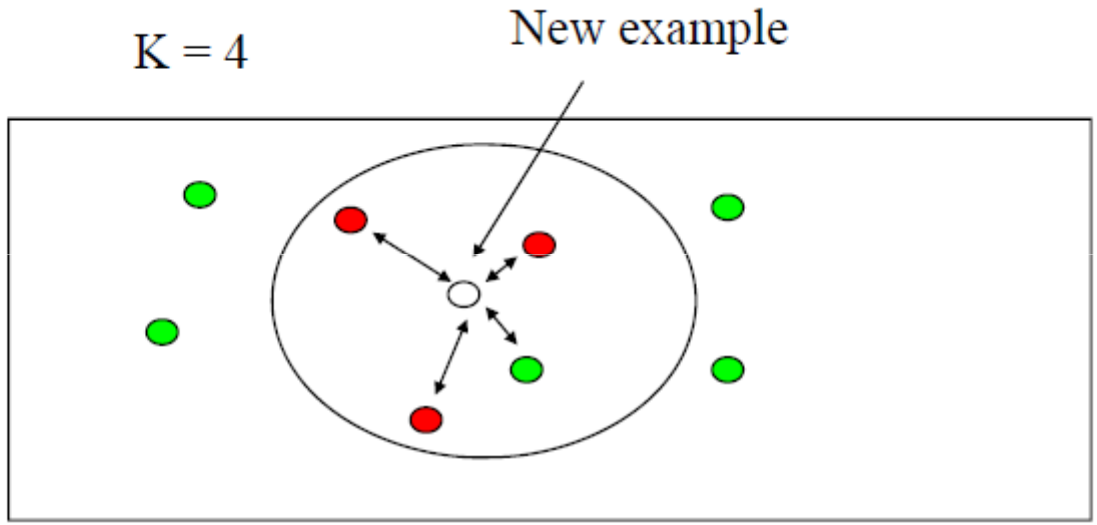


With large number of examples and possible noise in the labels, the decision boundary can become nasty!

We end up overfitting the data

K-Nearest Neighbor

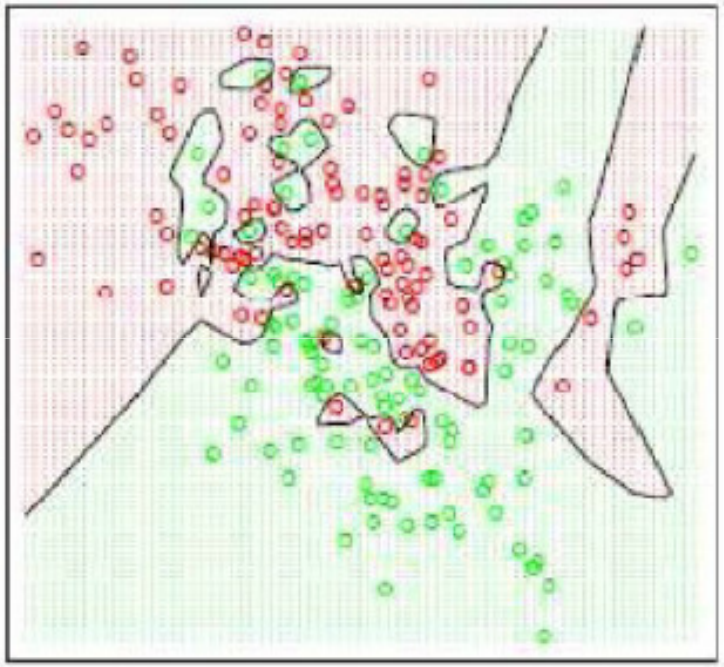
Example:



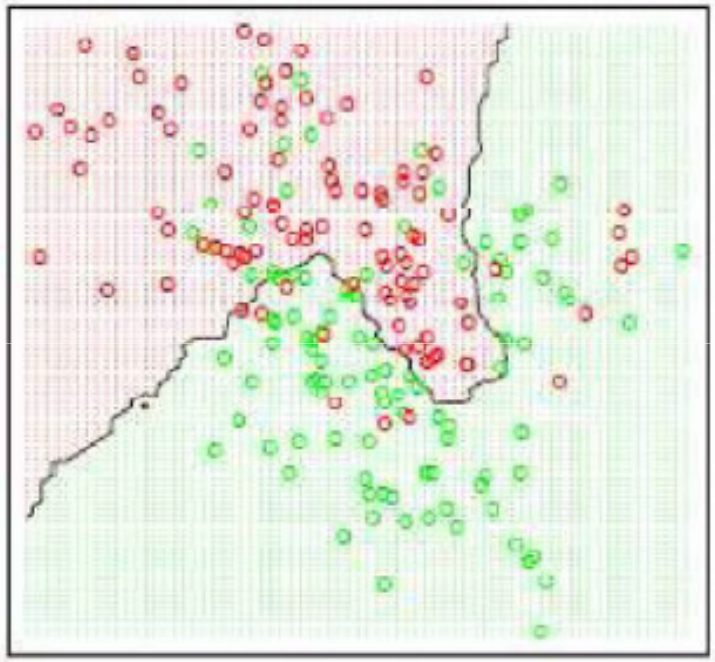
Find the ***k*** nearest neighbors and have them vote. Has a smoothing effect. This is especially good when there is noise in the class labels.

Effect of K

K=1



K=15



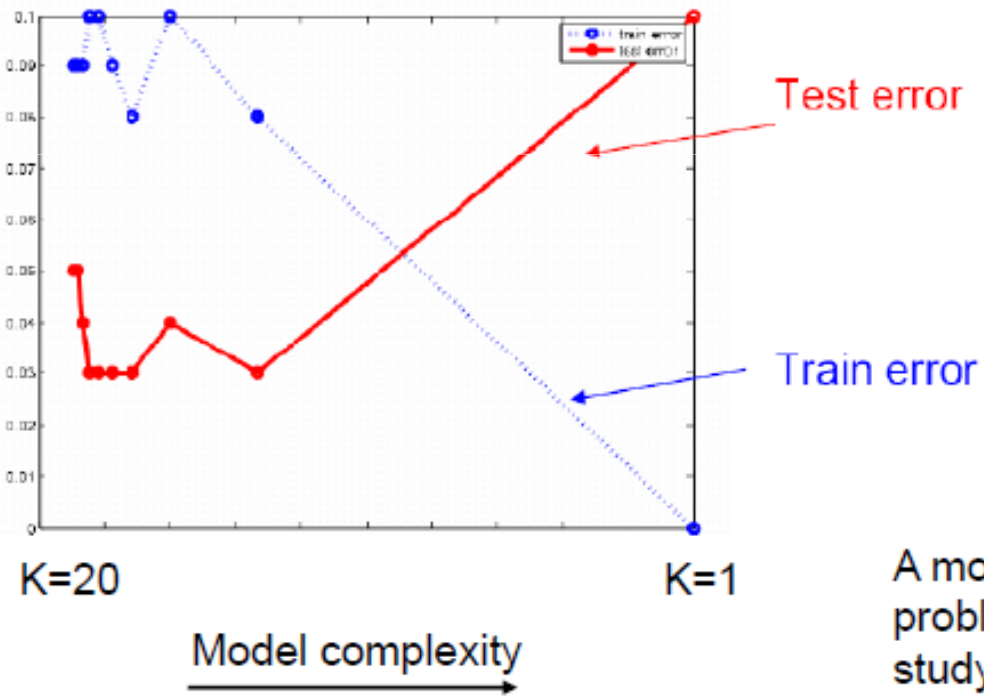
Figures from Hastie, Tibshirani and Friedman (Elements of Statistical Learning)

Larger k produces smoother boundary effect and can reduce the impact of class label noise.

But when K = N, we always predict the majority class

Question: how to choose k?

- Can we choose k to minimize the mistakes that we make on training examples (*training error*)?



A model selection problem that we will study later

Distance Weighted Nearest Neighbor

- It makes sense to weight the contribution of each example according to the distance to the new query example
  - Weight varies inversely with the distance, such that examples closer to the query points get higher weight
- Instead of only k examples, we could allow all training examples to contribute
  - Shepard's method (Shepard 1968)

Problems of k-NN

- Nearest neighbor is easily misled by noisy/irrelevant features

- One approach: Learn a distance metric:
  - that weights each feature by its ability to minimize the prediction error, e.g., its mutual information with the class.
  - that weights each feature differently or only use a subset of features and use cross validation to select the weights or feature subsets
  - Learning distance function is an active research area

Nearest Neighbor Summary

- Advantages
  - Learning is extremely simple and intuitive,
  - Very flexible decision boundaries
  - Variable-sized hypothesis space
- Disadvantages
  - distance function must be carefully chosen or tuned
  - irrelevant or correlated features have high impact and must be eliminated
  - typically cannot handle high dimensionality
  - computational costs: memory and classification-time computation
    - To reduce the cost of finding nearest neighbors, use data structure such as kd-tree