# COMP4388: **MACHINE LEARNING**

**Unsupervised learning – K-Means**

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## Unsupervised learning

- Supervised learning maps instances from an instance space x to an output space y using a set of labelled input instances
- Unsupervised learning, on the other hand, is the task of inferring/describing hidden structures or patterns from unlabelled data
- It is unsupervised as there is no class labels attached to the input instances

## Unsupervised learning

- Classification (or prediction or pattern detection) tasks result in a model that relates a set of input features to an output feature (i.e., target class). These models relate features to features and identify patterns within data
- Clustering (unsupervised) creates new data by assigning a cluster label from the set of unlabelled input feature vectors
- The label assigned to the cluster is inferred from the relationships within the data



## Clustering

- Clustering is an unsupervised machine learning task with the aim to divide data into clusters
- Clustering entails grouping data with similar properties together
- Used for Knowledge Discovery rather than prediction
- Can be seen as *Learning a new labelling function from unlabelled data*

## Clustering (2)

- Clustering is based on the concept that similar observations should have similar properties to each other and should be different from the observations outside that cluster (group)
- Related elements are grouped together



## Clustering (3)

- Useful to exemplify diverse data into much smaller number of groups
- This results in meaningful structures within data, which reduce complexity and provide insight into patterns of relationships among the groups

# Applications for Clustering

- Customer segmentation
  - Group customers with similar behaviours or similar demographics or even buying patterns for targeted marketing campaigns
- Anomaly detection
  - Detecting illegal or unauthorised intrusions into computer networks by identifying patterns outside the known patters



# Applications for Clustering (2)

- Social media
  - Clustering is used to determine communities of users. This is used, such as in Facebook, to refine advertising so that some ads go to certain groups of users
- Data simplification
  - Large datasets can be simplified by grouping large number of features with similar values into smaller number of homogeneous categories

## K-means clustering

- The most common clustering algorithm
- The basis of many more complicated clustering algorithms
- The *'k'* in the name is similar to the 'k' in kNN classifier!
- It assigns each of n input examples to k clusters
- k is the number of clusters (predefined; set by users)



## K-means clustering (2)

- Goal: Minimise the differences within each cluster and maximise the differences between clusters
- For each feature vector i, k-means assigns i to a cluster (initial guess) and then modifies the assignment to see changes in the homogeneity within clusters

## K-means clustering (3)

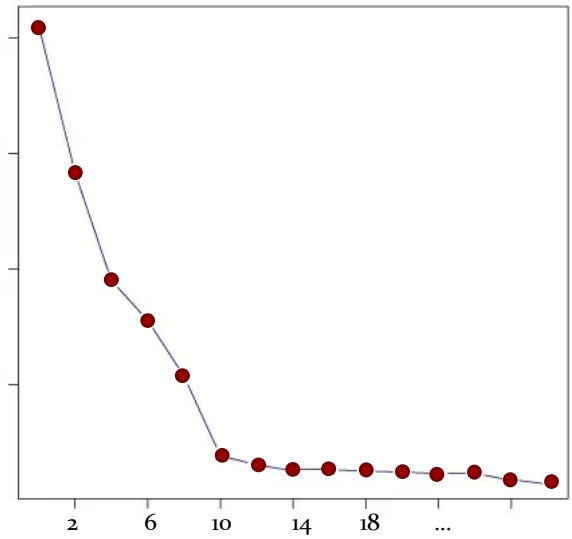
- Consists of two phases:
  - Assigns example to an initial set of k clusters
  - Updates the assignments by adjusting the cluster boundaries of each cluster based on the examples fall into each cluster
- This process is repeated until no improvement on the cluster
- The process is stopped and clusters are finalised



## K-means clustering (4)

- Similarly to kNN, k-means deals with data in multidimensional feature space
- The first step is to define the number of clusters
  - A quick rule-of-thump method is to select the sqrt(n/2) where n is number of data points in the dataset
  - One method to decide on the number of clusters is the Elbow Method
  - Select the number of clusters in which the Sum of Squared Error rate changes abruptly

# K-means clustering (4)






# K-means clustering (5)

- Each cluster has a centroid (referred to as mean as well)
- The centroid is a point to which the distance of the objects will be calculated
- Often, the points are chosen by selecting k random examples from the training set

## K-means clustering (6)

- Having chosen the initial cluster centres, new examples are assigned to the cluster centre that is nearest according to a distance function
- For a new input feature vector, the distance is computed with the centroids of all clusters and the new instance is assigned to the cluster with the minimal distance



## K-means clustering (7)

- Update step: the centroids of each cluster are re-calculated
- The new centroids are calculated as the average of the objects that belong to the cluster
- This is carried iteratively until there is no change in clusters

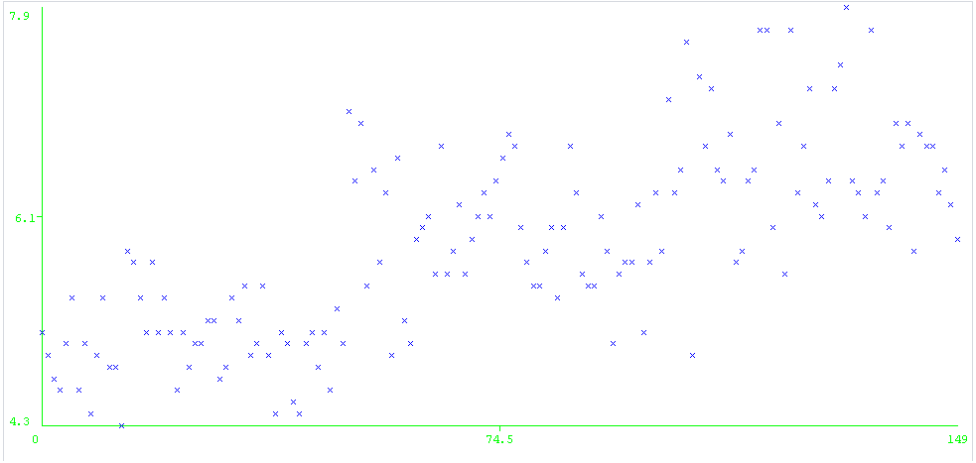
## Example: Iris Dataset

- The iris dataset consists of 150 number of training examples
- These are of three classes: Iris-setosa, Iris-verginica, Iris-versicolor
- Each feature vector consists of the following features: sepal width, sepal length, petal width, petal length



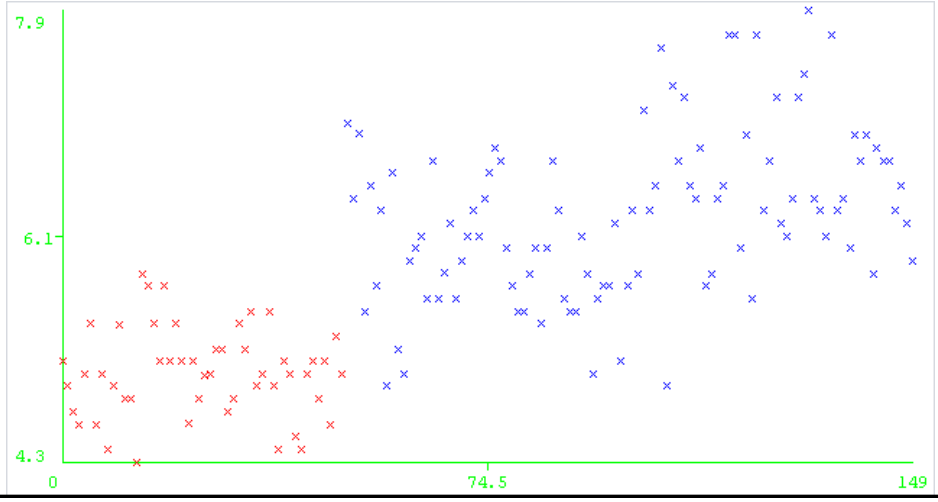
## Example: Iris Dataset

- Original Data



# Example: Iris Dataset

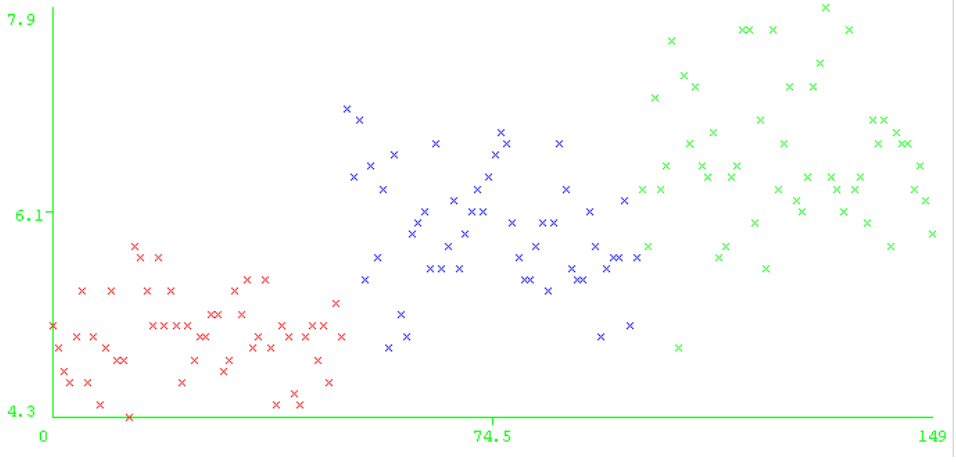
- Two clusters






# Example: Iris Dataset

- Three clusters



## Strengths of k-means

- Based on an easy to understand and simple principle for identifying clusters
- Flexible and adjustable
- Efficient and performs well at dividing the data into useful clusters



## Weaknesses of k-means

- Less sophisticated than more recent clustering algorithms
- Based on a random chance, which does not guarantee the algorithm to find the optimal set of clusters
- Requires reasonable guesses as to how many clusters naturally exist in the data