Machine Learning for Economics and Finance 1
K means clustering

Kien C Nguyen

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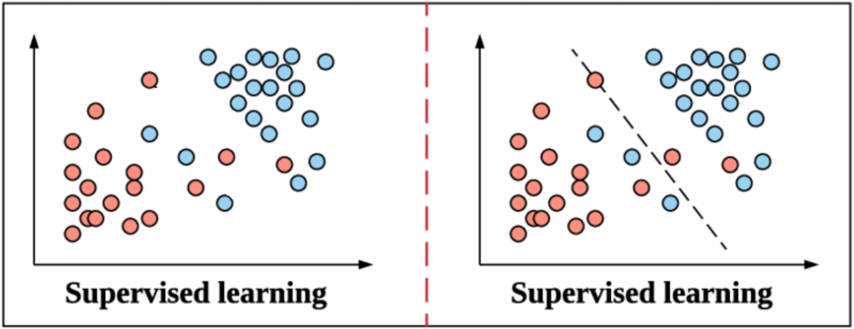
Introduction - Supervised Learning

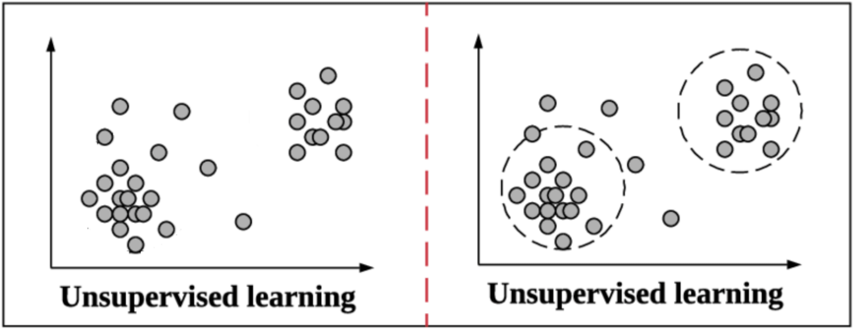
1. Supervised Learning
   - Input : data X and label Y
   - Goal : find parameters w that minimize the loss function
2. Why Supervised Learning?
   - predict outcomes from previous experiences

Figure: Supervised Learning (Source: Orchestrating Development Lifecycle of Machine Learning Based IoT Applications: A Survey, Zhenyu Wen)



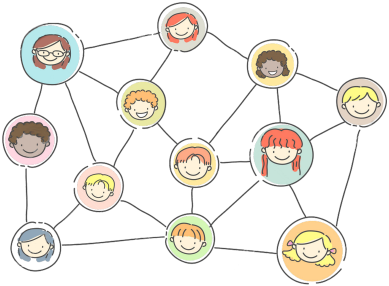
1. Unsupervised Learning
   - Input : data X
   - Goal : group data by finding some commonality in the features
2. Why Supervised Learning?
   - find features which can be useful for categorization
   - find all kind of unknown patterns in data

Figure: Unsupervised Learning



Introduction - Applications

- Spam email filter
- Marketing and Sales
- Social Network



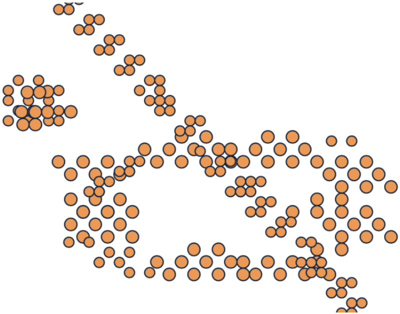
Introduction - Clustering

- Input : $S = \{x^{(i)}\}_{i=1}^{N}$ (N: number of samples), each sample (data point) is a D-dimensional vector

$$x^{(i)} = (x_1^{(i)}, x_2^{(i)}, \ldots, x_D^{(i)})^T$$

- Output: find structure in the data and organize them into groups.

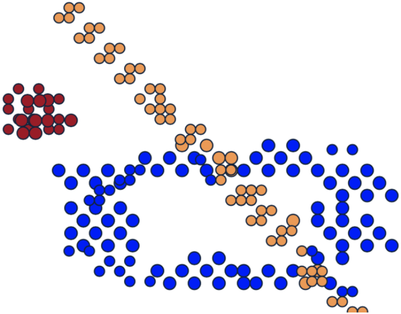
Figure: Input samples. (Source: UIUC CS446 Lecture notes [1])



Introduction - Clustering

- A cluster is a set of samples that are alike
- Samples in different clusters are not alike

Figure: Clustered input samples. (Source: UIUC CS446 Lecture notes [1])



Distance Measures

- A distance measure (metric) is a function $d : R^D \times R^D \to R$ that satisfies
  1. $d(\mathbf{x}, \mathbf{y}) \geq 0, \quad d(\mathbf{x}, \mathbf{y}) = 0 \Leftrightarrow \mathbf{x} = \mathbf{y}$
  2. $d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z}) \geq d(\mathbf{x}, \mathbf{z})$ (Triangle inequality)
  3. $d(\mathbf{x}, \mathbf{y}) = d(\mathbf{y}, \mathbf{x})$ (Symmetry)
- For the purpose of clustering, sometimes we can use distances that are not a metric (e.g. those that do not satisfy triangle inequality or symmetry.)

Distance Measures

- L^2 distance (Euclidean distance)

$$\begin{aligned} d(\mathbf{x},\mathbf{y}) &= \|(\mathbf{x}-\mathbf{y})\|_2 = \sqrt{(\mathbf{x}-\mathbf{y})^2} \\ &= \sqrt{(\mathbf{x}-\mathbf{y})^T(\mathbf{x}-\mathbf{y})} = \sqrt{\sum_{i=1}^{D}(x_i-y_i)^2} \end{aligned}$$

- L^1 distance (Manhattan distance)

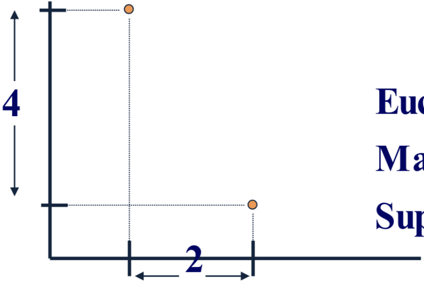
$$d(\mathbf{x},\mathbf{y}) = \|(\mathbf{x}-\mathbf{y})\|_1 = \sum_{i=1}^{D}|x_i-y_i|$$

- L^∞ distance (sup distance)

$$d(\mathbf{x},\mathbf{y}) = \|(\mathbf{x}-\mathbf{y})\|_\infty = max_{1\le i\le D}|x_i-y_i|$$

Distance measures

Figure: Different types of distance measures. (Source: UIUC CS446 Lecture notes [1])



$$\textbf{Euclidean} = (4^2 + 2^2)^{1/2} = 4.47$$

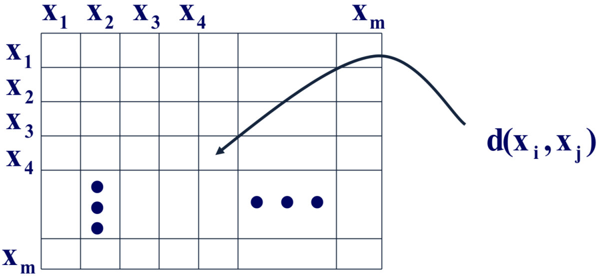
$$\textbf{Manhattan}: 4 + 2 = 6$$

$$\textbf{Sup} = \text{Max}(4,2) = 4$$

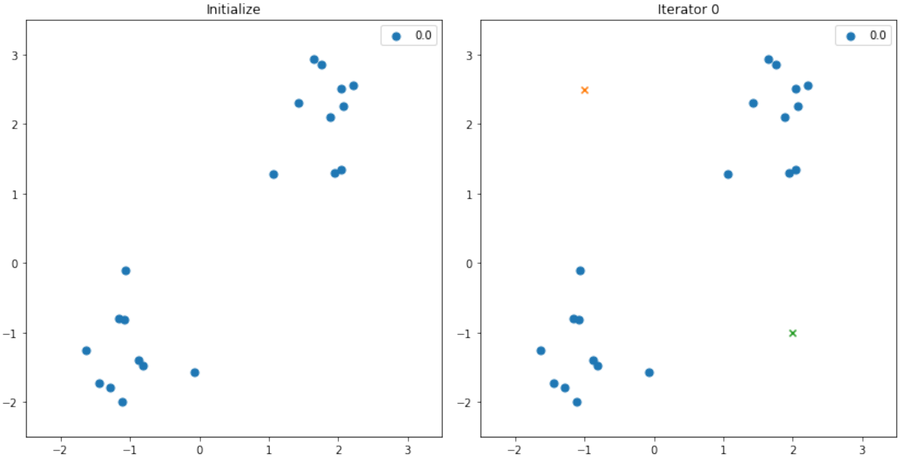
Distance measures

- We are given a matrix of distances between any pair of samples.

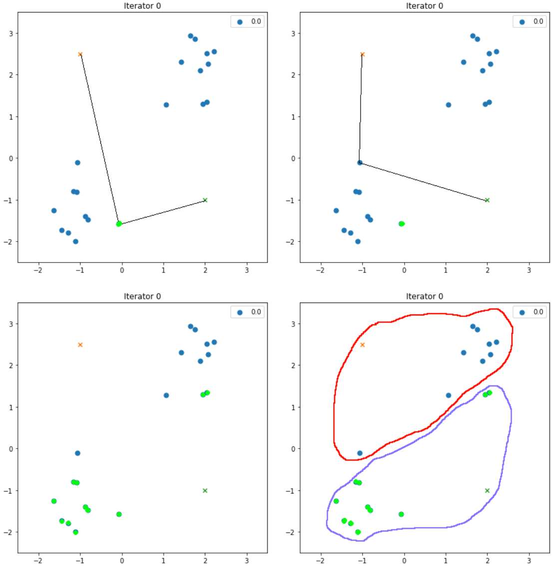
Figure: Matrix of distances. (Source: UIUC CS446 Lecture notes [1])



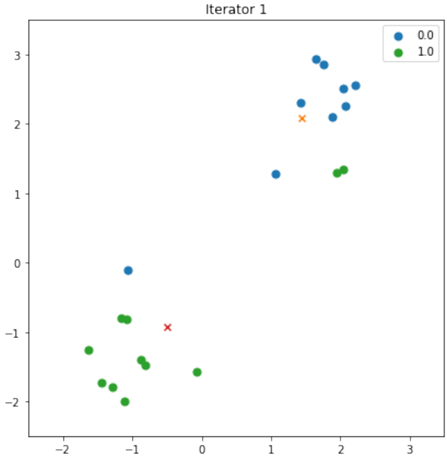
K-means Algorithm



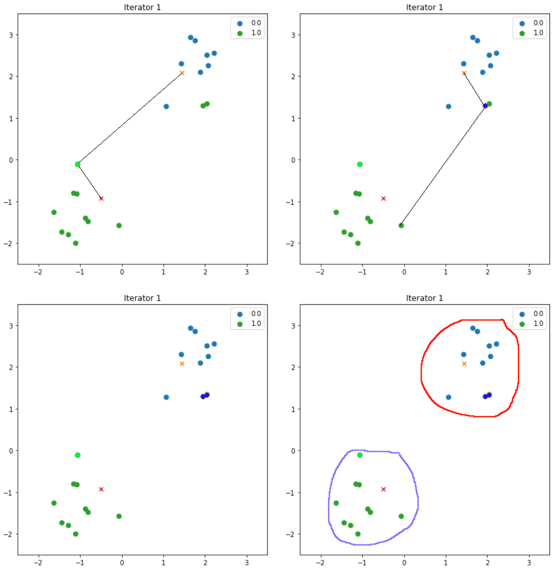
K-means Algorithm



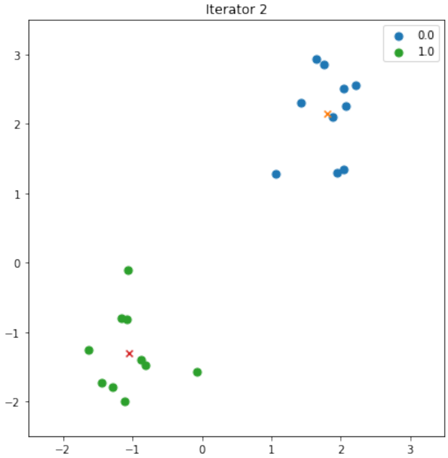
K-means Algorithm



K-means Algorithm



K-means Algorithm



Input:

- K (number of clusters)
- $\{x^{(i)}\}_{i=1}^{N}$

Initialization:

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^D$

while *Assignment changes from the last iteration* **do**

  Assignment:

  for *i = 1 to N* **do**

    Assign $x^{(i)}$ to the cluster with the minimum distance $d(x^{(i)}, \mu_k)$

  end

  Update:

  for *j=1 to K* **do**

    μ_k = mean of all the points assigned to cluster k

  end

end

Algorithm 1: K-means Algorithm

Challenges of K-means

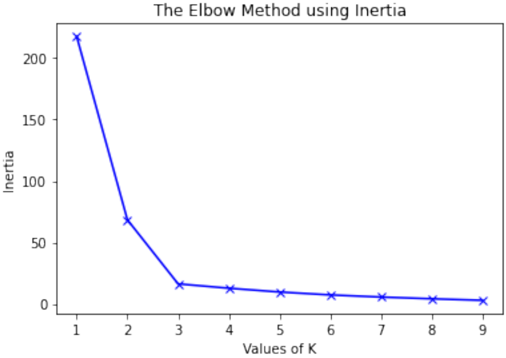
- Different K different outputs.
- With same K, the output won't be always the same because of the randomly initial centroids.
- Due to the nature of Euclidean distance, it is not a suitable algorithm when dealing with clusters that adopt non-spherical shapes.

How to choose right K

- Field knowledge
- Business decision
- Elbow Method

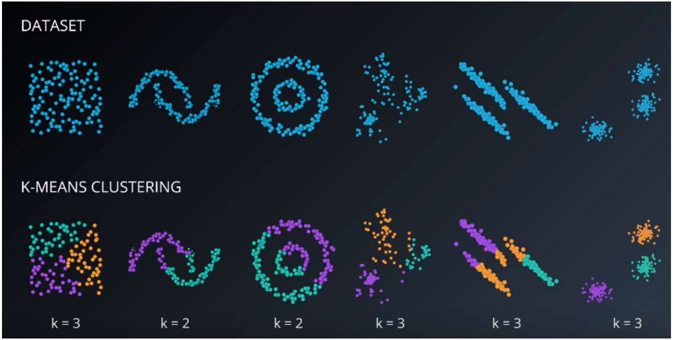
Elbow Method

- The elbow method is used for determining the correct number of clusters in a dataset.
- How it works? Plot the cost function against K and choose K using the "elbow" method.



K-means Limitations

- K-means clustering with spherical-shaped distributions



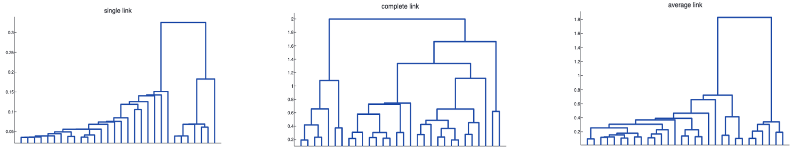
Main approaches:

- Bottom-up/Agglomerative clustering: each data point starts in its own cluster
- Top-down/Divisive clustering: all data points start in the same cluster

Input:
$\{x^{(i)}\}_{i=1}^{N}$
Initialization:
Clusters as singletons C_i for $i \in \{1, ..., N\}$ and set of clusters available for merging $S \leftarrow \{1, ..., n\}$
while *There are available clusters for merging* **do**
  Pick 2 most similar clusters to merge: $(j, k) \leftarrow_{j,k \in S} d_{j,k}$
  Create new cluster $C_{l_j} \cup C_k$
  Mark j and k as unavailable: $S \leftarrow S \setminus \{j, k\}$
  if $C_l \neq \{1, ..., N\}$ **then**
    Mark l as available, $S \leftarrow S \cup \{l\}$
  end
  Update:
  for $i \in S$ **do**
    Update dissimilarity matrix $d(i, l)$
  end
end

Algorithm 2: Agglomerative clustering

Different variants of agglorative clustering:



(a) Single linkage (b) Complete linkage (c) Average linkage

Figure: Hierarchical clustering of yeast gene expression data

Single link	Complete link	Average link
$min_{i \in G, j \in H} d_{i,j}$	$max_{i \in G, j \in H} d_{i,j}$	$\frac{1}{N_G N_H} \sum_{i \in G} \sum_{j \in H} d_{i,j}$

Table: Distance between two clusters $d(G, H)$

Hierarchical Clustering - Advantages vs Disadvantages

- No need of defining K - number of clusters
- Easy to implement and the dendrogram produced is very useful in understanding the data
- Time complexity $O(nlogn)$ (compare with k-Mean)
- Sensitivity to noise and outliers, breaking large clusters, difficulty handling different sized clusters and convex shapes
- No backtracking, No object function

Other Unsupervised Learning Algorithms

- Density-Based Spatial Clustering of Applications with Noise (DBSCAN)
- Gaussian Mixture Models (GMM)
- Principal Component Analysis (PCA)

References

[1] UIUC CS 446 Machine Learning
[2] Andrew Ng – Coursera's Machine Learning
[3] https://towardsdatascience.com/unsupervised-machine-learning-clustering-analysis-d40f2b34ae7e
[4] K. P. Murpy – Machine Learning – A Probabilistic Perspective, MIT Press, 2012
[5] VEF Academy – Machine Learning, 2018-2020
[6] VEF Academy – Fundamentals of Machine Learning, 2020