

W5. Unsupervised Learning - Clustering & PCA

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Week 5

Motivation

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- This returns poor accuracy, and you feel terrible and start thinking of some strategic method to find a few important variables.
- That's where Principal Component Analysis (PCA) is used.

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- PCA is often used in the preliminary data analytics, before running any machine learning tasks.

How PCA works

- Consider a matrix X with N rows (aka "observations") and K columns (aka "variables").

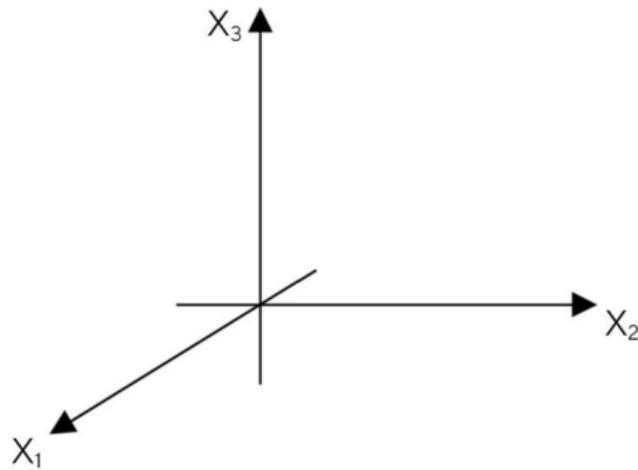
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- Each variable represents one coordinate axis. For each variable, the length has been standardized according to a scaling criterion, normally by scaling to unit variance.

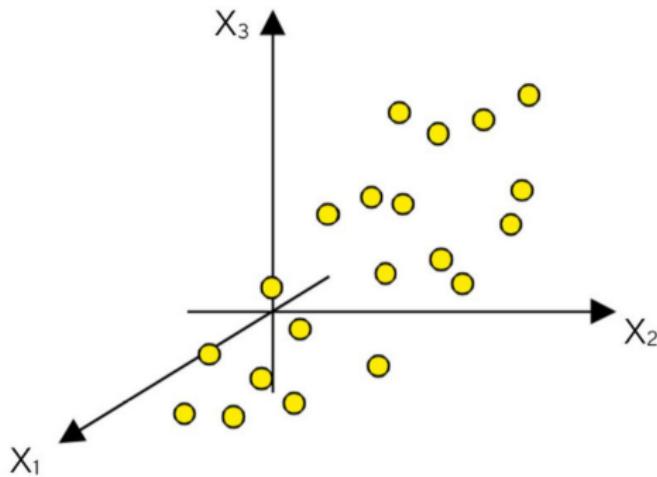
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- A K-dimensional variable space. For simplicity, only three variables axes are displayed. The “length” of each coordinate axis has been standardized according to a specific criterion, usually unit variance scaling.

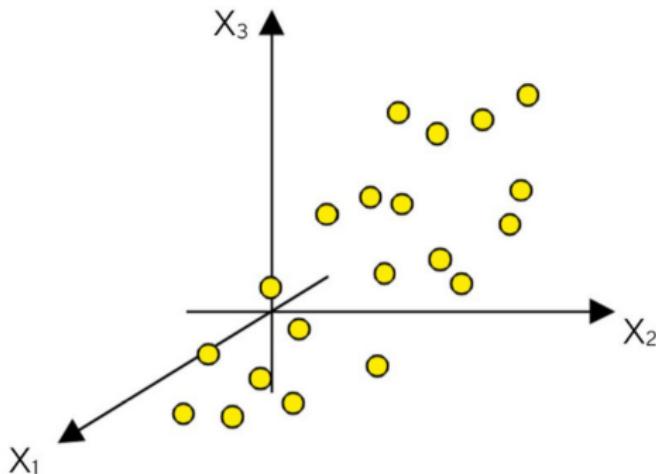
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- In the next step, each observation (row) of the X -matrix is placed in the K -dimensional variable space. Consequently, the rows in the data table form a swarm of points in this space.



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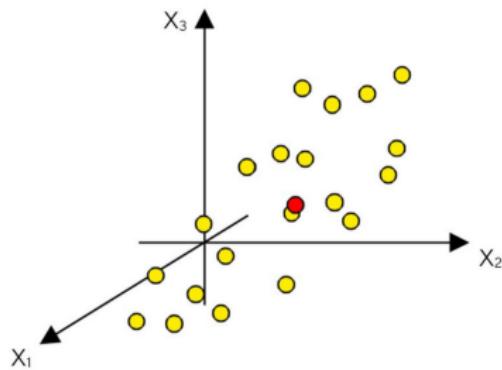
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- The observations (rows) in the data matrix X can be understood as a swarm of points in the variable space (K -space).

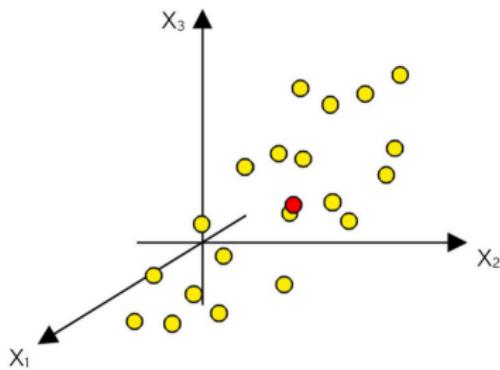
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- Next, mean-centering involves the subtraction of the variable averages from the data. The vector of averages corresponds to a point in the K -space.



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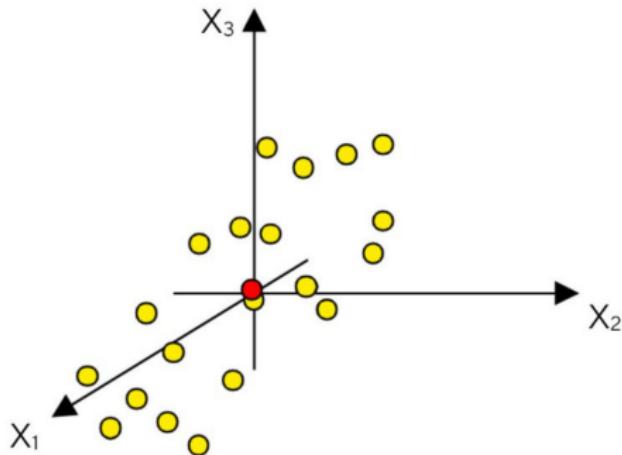
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- In the mean-centering procedure, you first compute the variable averages. This vector of averages is interpretable as a point (here in red) in space. The point is situated in the middle of the point swarm (at the center of gravity).

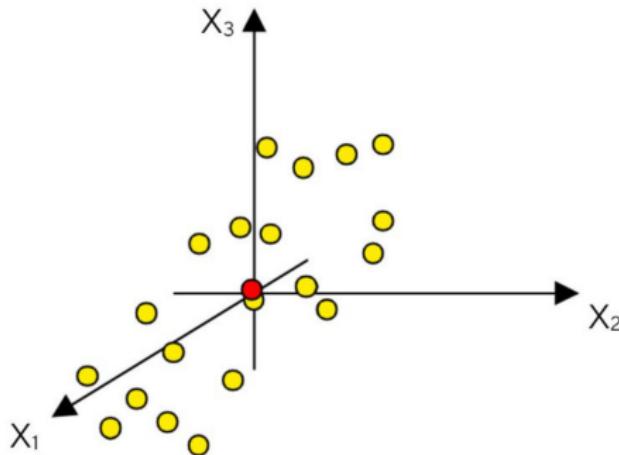
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- The mean-centering procedure corresponds to moving the origin of the coordinate system to coincide with the average point (here in red).

The first principal component

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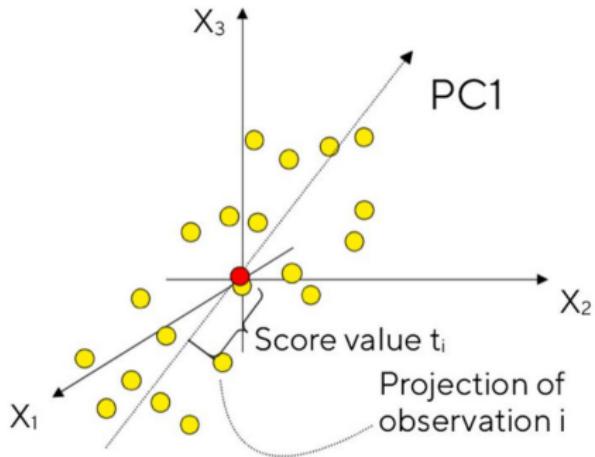
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- Each observation (yellow dot) may now be projected onto this line in order to get a coordinate value along the PC-line. This new coordinate value is also known as the score.

The first principal component



- The first principal component (PC1) is the line that best accounts for the shape of the point swarm. It represents the *maximum variance direction* in the data.

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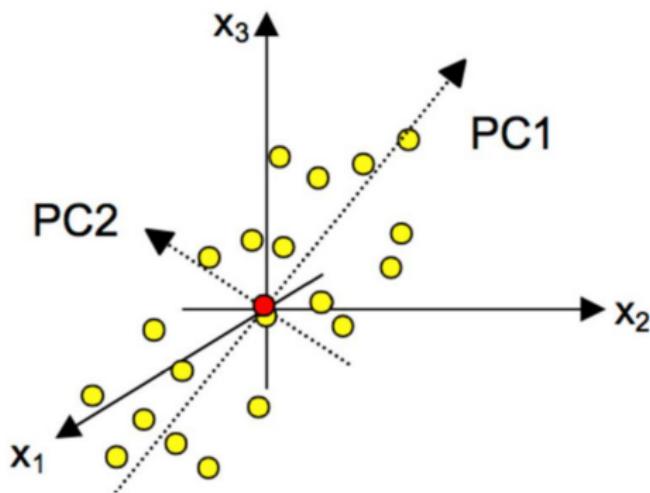
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- This line also passes through the average point.

The second principal component



- The second principal component (PC2) is oriented such that it reflects the second largest source of variation in the data while being *orthogonal* to the first PC. PC2 also passes through the average point.

How to calculate the PC1 and PC2 ?

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- **Standardize the data:** Ensure that each feature has a mean of 0 and a standard deviation of 1. This is important for PCA because it is sensitive to the scales of the variables.
- **Calculate the covariance matrix:** The covariance matrix is a square matrix that captures the covariance between each pair of features in the dataset. The covariance matrix (with dimension $k \times k$) is

$$\hat{\Sigma} = \frac{1}{n-1} X^T X,$$

where X is the standardized data matrix (dimnesion $n \times k$) with n observations and k features.

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- The eigenvectors $\{v_1, v_2, \dots, v_k\}$ and eigenvalues $\{\lambda_1, \lambda_2, \dots, \lambda_k\}$ are the set of vectors/values such that

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- The eigen-decomposition of $\hat{\Sigma}$ can be written as

$$\hat{\Sigma} = V \Lambda V^T,$$

where V is a matrix containing the eigen-vectors and Λ is a diagonal matrix with diagonal elements as eigenvalues.

How to calculate the PC1 and PC2 ?

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- **Sort the eigenvectors by their corresponding eigenvalues in descending order:** The eigenvector associated with the largest eigenvalue is the first principal component, and the eigenvector associated with the second largest eigenvalue is the second principal component.
- Then PC1 and PC2 can be represented as

$$PC1 = v_1$$

$$PC2 = v_2$$

where v_1 and v_2 are the eigenvectors corresponding to the largest and second largest eigenvalues, respectively.

Two principal components define a model plane

- When two principal components have been derived, they together define a place, a window into the K-dimensional variable space.

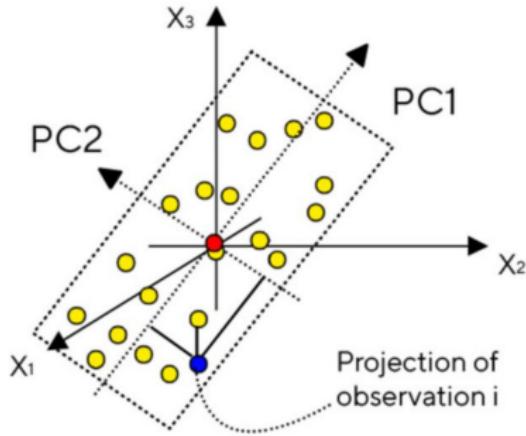
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- By projecting all the observations onto the low-dimensional sub-space and plotting the results, it is possible to visualize the structure of the investigated data set.
- The coordinate values of the observations on this plane are called scores, and hence the plotting of such a projected configuration is known as a score plot.

Two principal components define a model plane



- Two PCs form a plane. This plane is a window into the multidimensional space, which can be visualized graphically. Each observation may be projected onto this plane, giving a **score** for each.

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- Here, the first column of T contains the scores for the first principal component (PC1), the second column contains the scores for the second principal component (PC2), and so on.

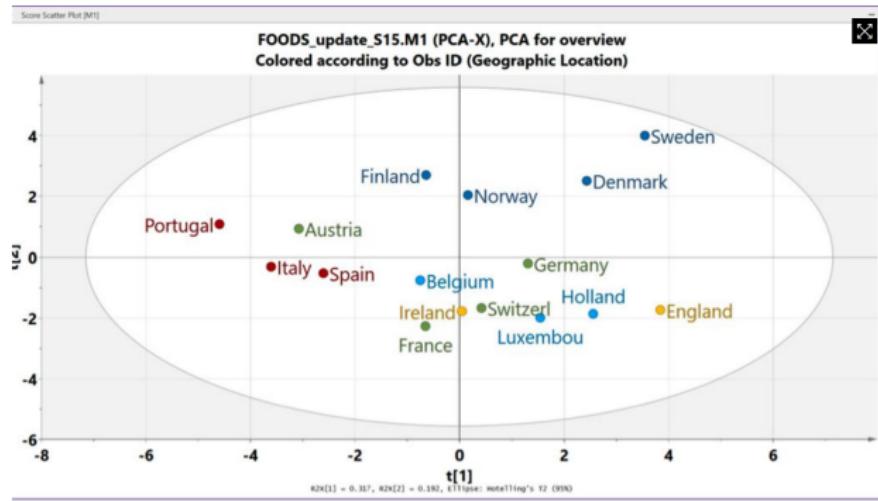
A real example to model a dataset

- Now, let's consider what this looks like using a data set of foods commonly consumed in different European countries. The figure in the next page displays the score plot of the first two principal components. These scores are called t_1 and t_2 .

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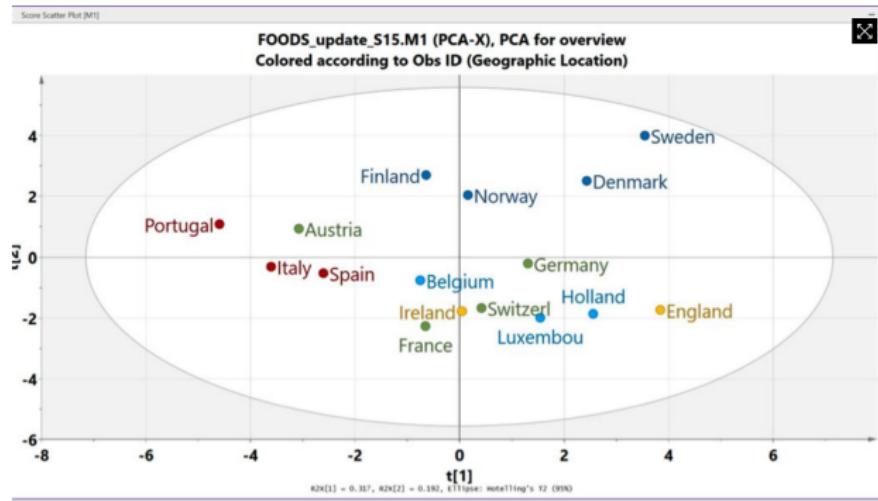
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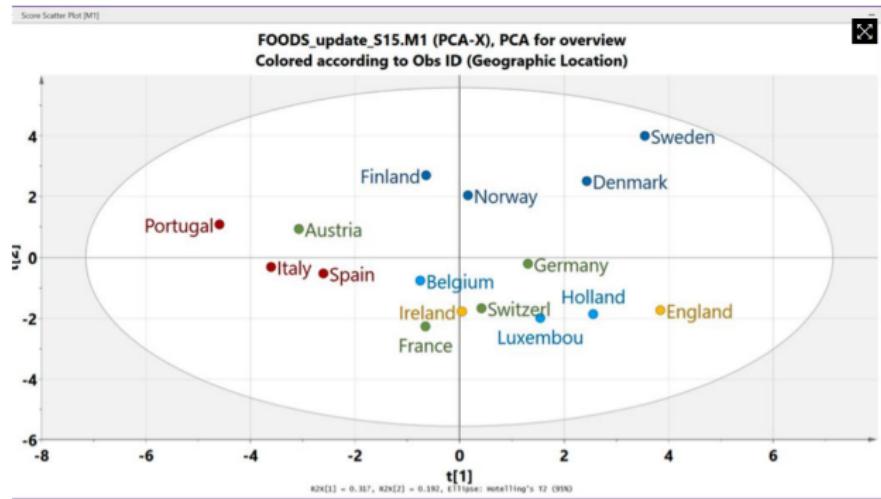
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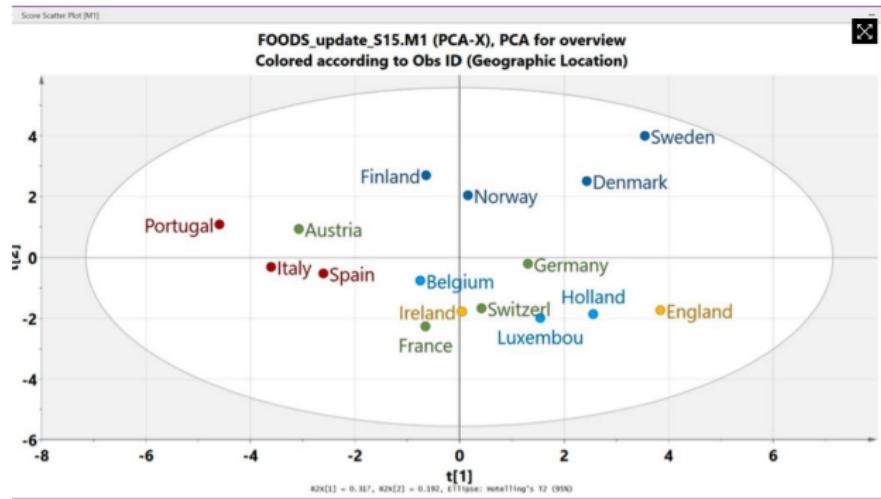
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- The first component explains 32% of the variation, and the second component 19%.

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- Belgium and Germany are close to the center (origin) of the plot, which indicates they have average properties.

Exercise: PCA

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 - Calculate the scores:** Project the centered data onto the principal component(s).

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- Find the eigenvalues and eigenvectors:

- eigenvalues : 0,8
- eigenvectors:

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- Calculate the scores: Project the centered data onto the principal component: Scores = Centered data \times Principal component =
$$\begin{bmatrix} -2\sqrt{2} & 0 \\ 0 & 0 \\ 2\sqrt{2} & 0 \end{bmatrix}$$

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- Need for Robust PCA: To address the limitations of standard PCA, Robust PCA was developed.
- Unlike standard PCA, Robust PCA is designed to separate the low-rank structure of the data (representing the true signal) from the sparse noise or outliers. This makes it more suitable for real-world datasets that are often corrupted by noise or contain anomalies.

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- The L-1 norm of a matrix A is defined as the sum of the absolute values of all its entries.

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- Certainly not! It is a manual process and will take a huge amount of time.
- So what can the bank do?

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- The bank can now make three different strategies or offers, one for each group, instead of creating different strategies for individual customers.
- Note that “high income,” “average income,” “low income” are not pre-specified labels, but the outcome of clustering. So, this is un-supervised learning.

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- Here, we are given feature vectors for each data point $x^{(i)} \in \mathbb{R}^n$ as usual; but no labels $y^{(i)}$ (making this an unsupervised learning problem).
- Our goal is to predict k centroids and a label " $c^{(i)}$ " (corresponding to different clusters) for each datapoint. The k-means clustering algorithm is as follows:

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 - (1) assigning data points to clusters based on the current centroids

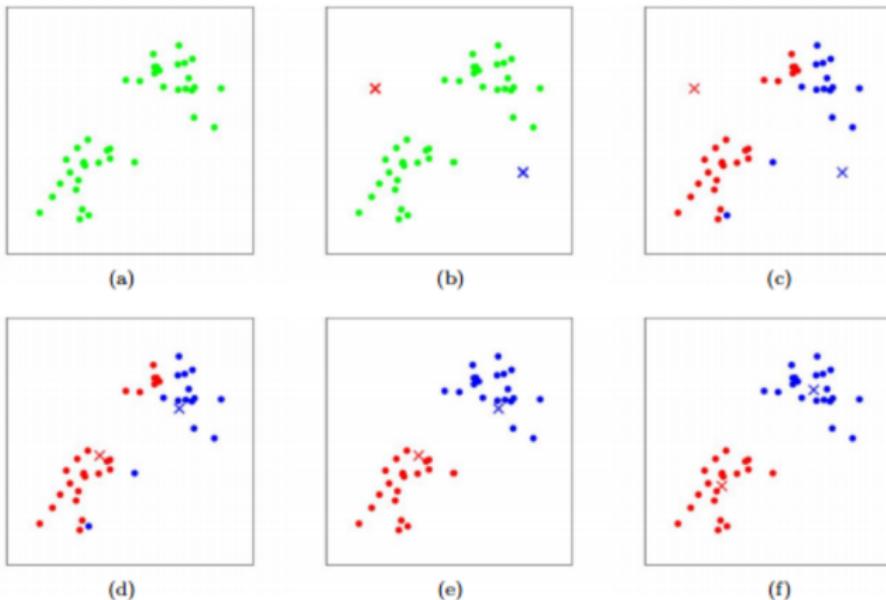
K-Means

- K-Means is one of the most popular "clustering" algorithms.
- K-Means stores k centroids that it uses to define clusters. A point is considered to be in a particular cluster if it is closer to that cluster's centroid than any other centroid.
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- The value of K is often pre-specified.

K-Means



- Training examples are shown as dots, and cluster centroids are shown as crosses.

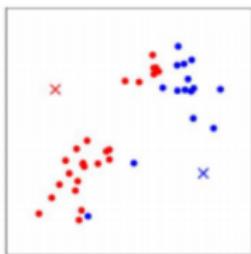
K-Means



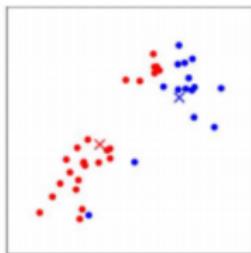
(a)



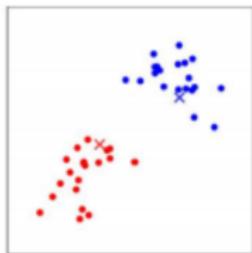
(b)



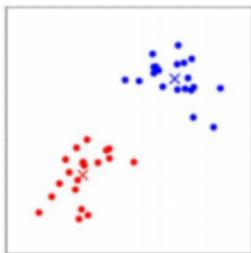
(c)



(d)



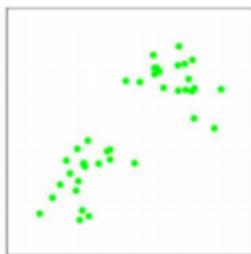
(e)



(f)

- (a) Original dataset.

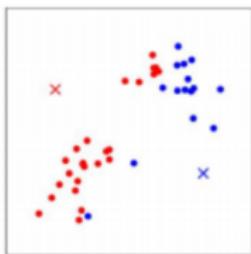
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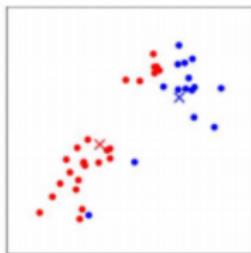
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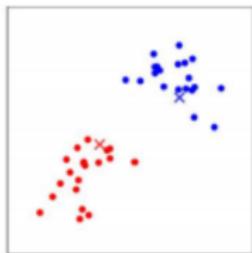
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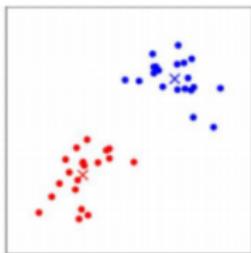
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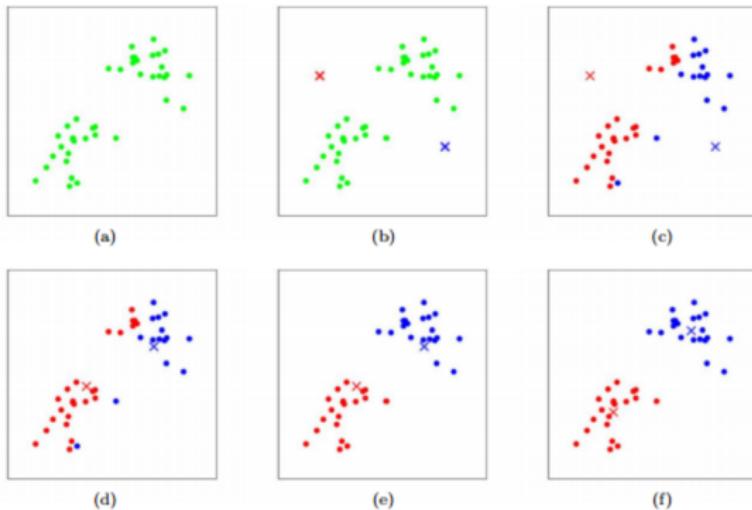
(e)



(f)

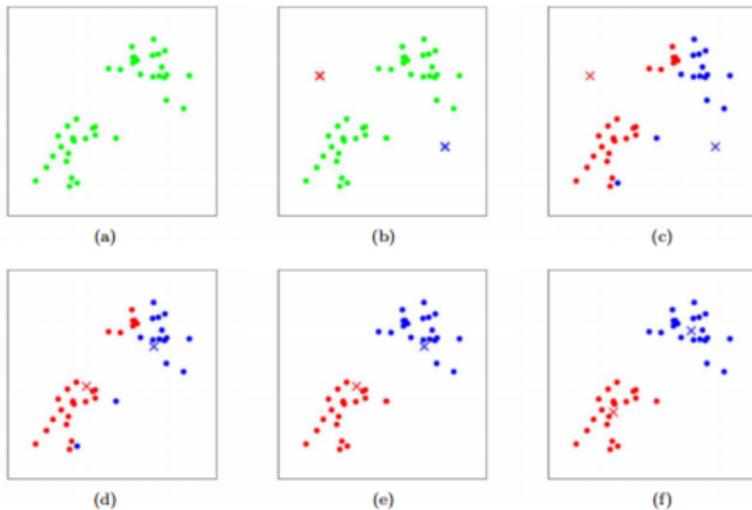
- (b) Random initial cluster centroids.

K-Means



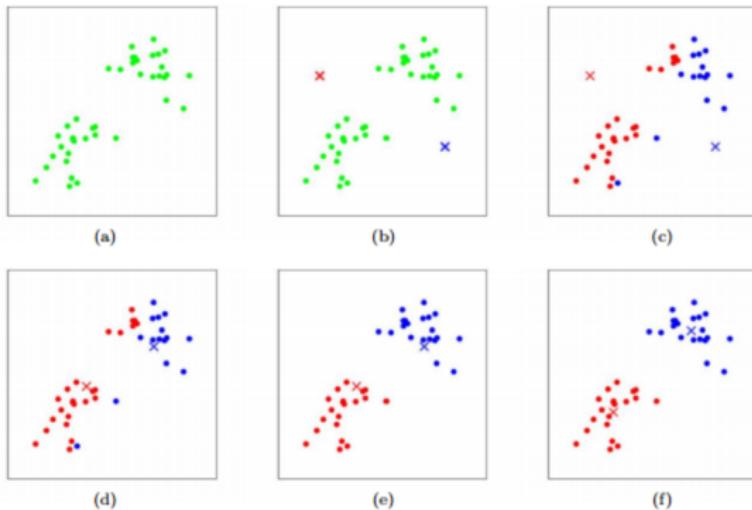
- (c-f) Illustration of running two iterations of k-means.

K-Means



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- Then we move each cluster centroid to the mean of the points assigned to it.

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 - (4) Repeat Steps 2 and 3 and provide the clusters and centroids for 2 iterations.

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 - New Centroids: Centroid 1: (1.5, 1), Centroid 2: (3.5, 3.667)

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- Unlike k-means, where each data point belongs to exactly one cluster, FCM introduces the concept of membership levels, allowing data points to have varying degrees of belonging to multiple clusters.

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- Each data point x_i has a degree of membership u_{ij} in each cluster j , where u_{ij} is a number between 0 and 1 representing the degree to which x_i belongs to cluster j .

Fuzzy C-Means clustering

- The FCM algorithm aims to minimize the following objective function:

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- $\|x_i - v_j\|$ is the Euclidean distance between the data point x_i and the cluster center v_j .

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- The algorithm stops when the changes in the membership matrix between consecutive iterations are below a specified threshold.

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- Suppose we have a dataset with four points: A, B, C, and D. We want to cluster these points into two clusters using Fuzzy C-means. After running the algorithm, we might get the following membership values for each point in each cluster:

Point	Cluster 1	Cluster 2
A	0.8	0.2
B	0.3	0.7
C	0.6	0.4
D	0.1	0.9

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- Point D has a very low membership value (0.1) in Cluster 1 and a high value (0.9) in Cluster 2, showing that it is strongly associated with Cluster 2.

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Fuzzy C-Means clustering

- Advantages

- 1) Gives best result for overlapped data set and comparatively better than k-means algorithm.
- 2) Unlike k-means where data point must exclusively belong to one cluster center, here data point is assigned membership to each cluster center as a result of which data point may belong to more than one cluster center.

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Fuzzy C-Means clustering

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 - 1) Apriori specification of the number of clusters.
 - 2) Euclidean distance measures can unequally weight underlying factors.