W9. Unsupervised Learning - Clustering & PCA

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Week 9

Motivation

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- 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.

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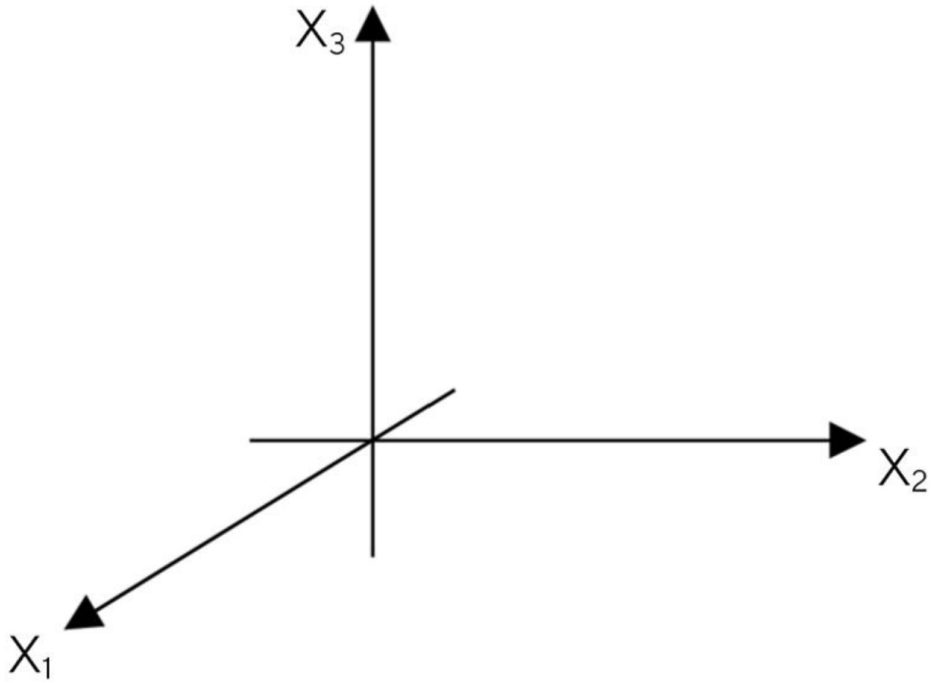
- Each variable represents one coordinate axis. For each variable, the length has been standardized according to a scaling criterion, normally by scaling to unit variance.

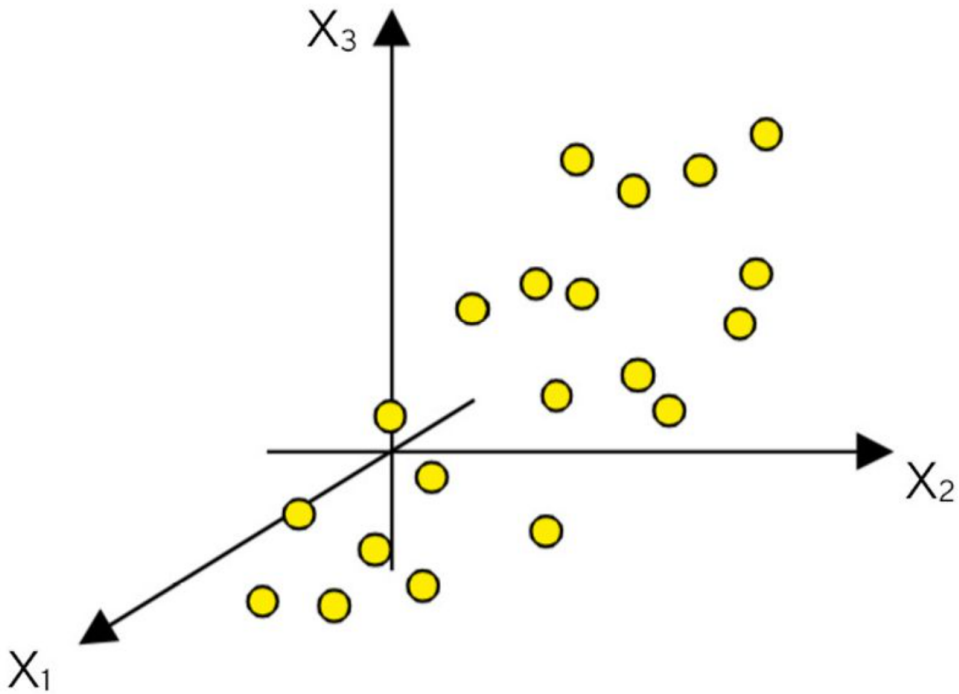
How PCA works



- 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.

How PCA works

- 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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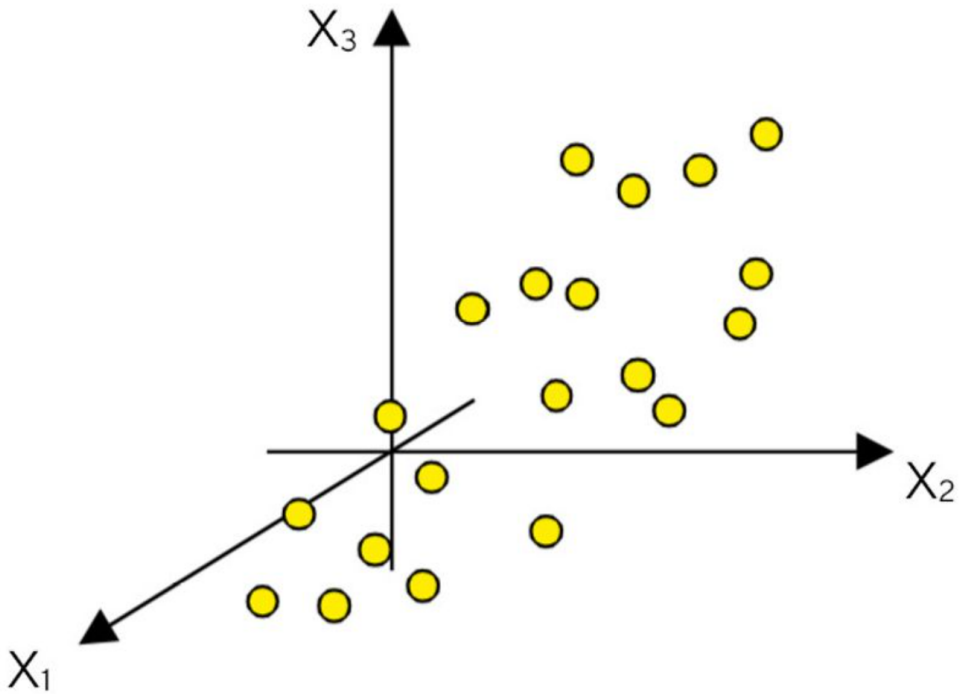

- The observations (rows) in the data matrix X can be understood as a swarm of points in the variable space (K-space).

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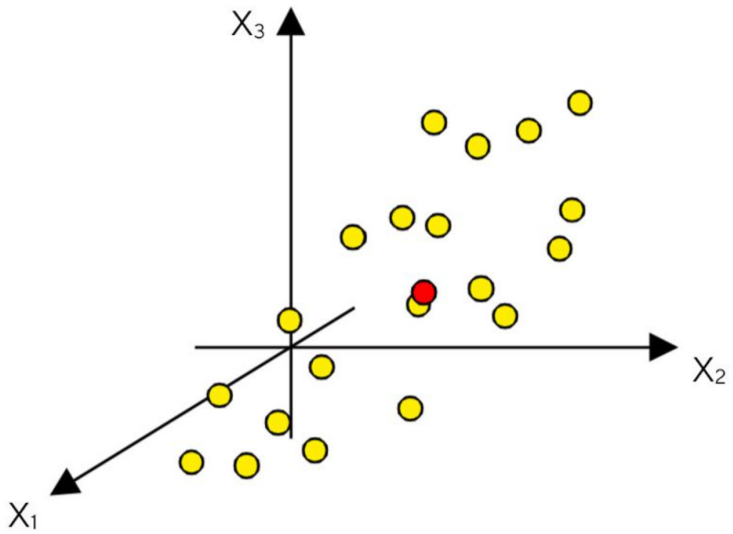
- Next, mean-centering involves the subtraction of the variable averages from the data. The vector of averages corresponds to a point in the K-space.



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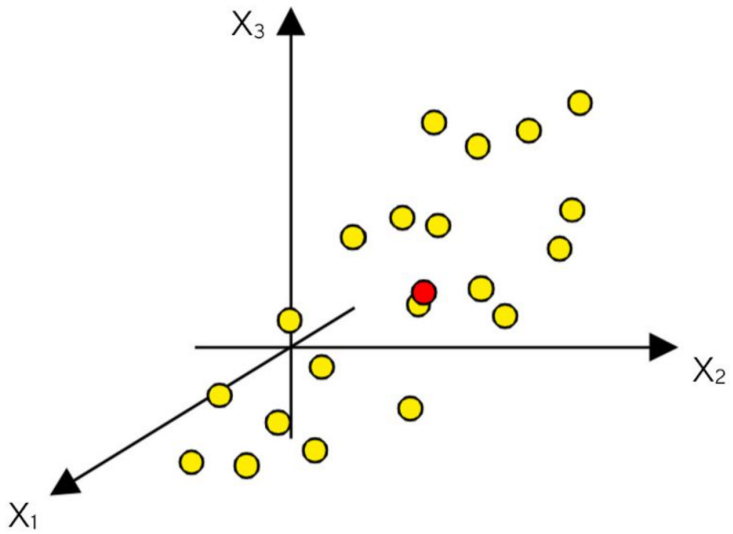
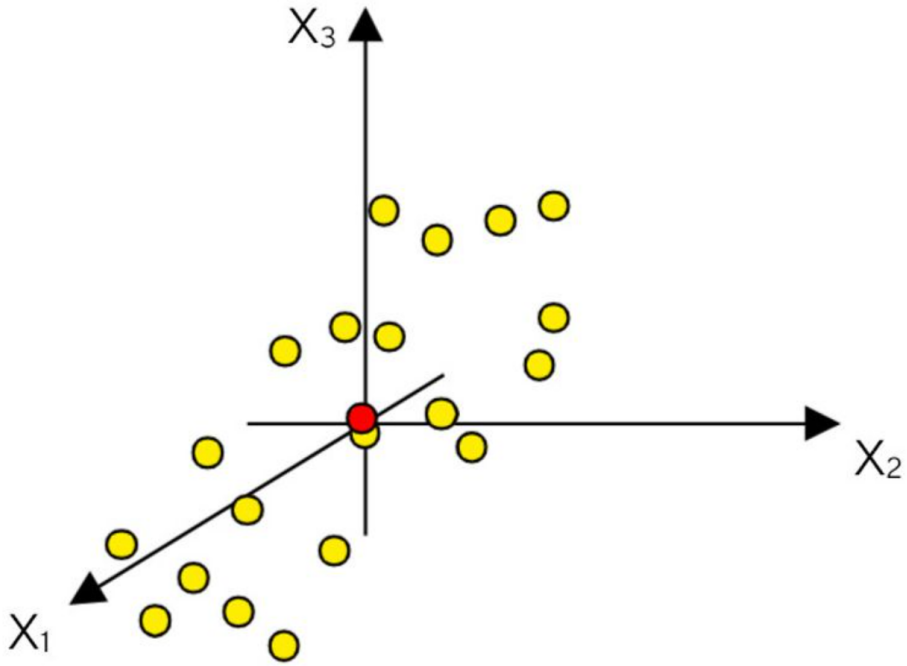


- In the mean-centering procedure, you first compute the variable averages. This vector of averages is interpretable as a point (here in red) in space. The point is situated in the middle of the point swarm (at the center of gravity).

How PCA works

- The subtraction of the averages from the data corresponds to a re-positioning of the coordinate system, such that the average point now is the origin.



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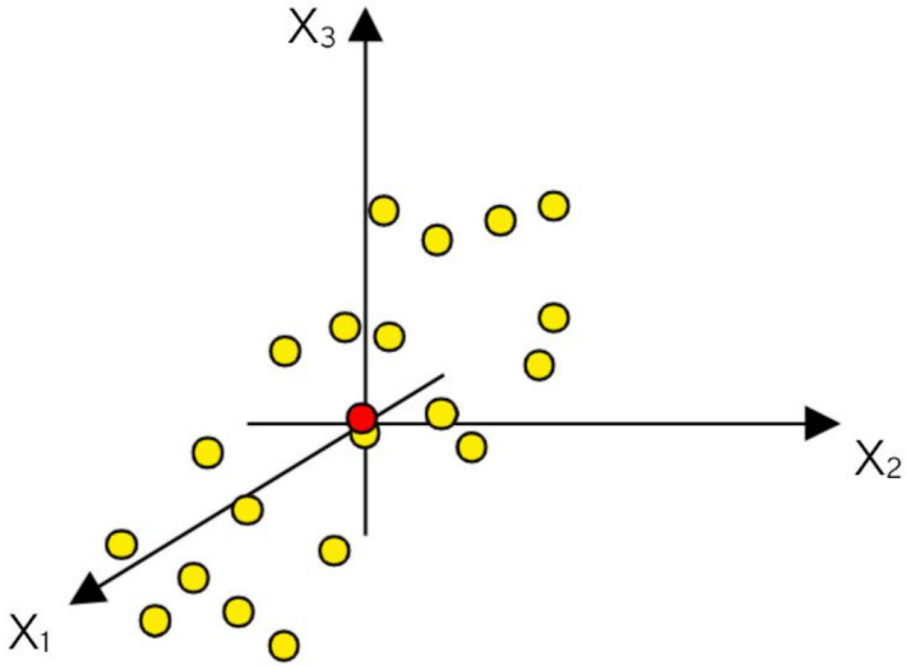

- The mean-centering procedure corresponds to moving the origin of the coordinate system to coincide with the average point (here in red).

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- This component is the line in the K-dimensional variable space that best approximates the data in the least squares sense. This line goes through the average point.
- 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.

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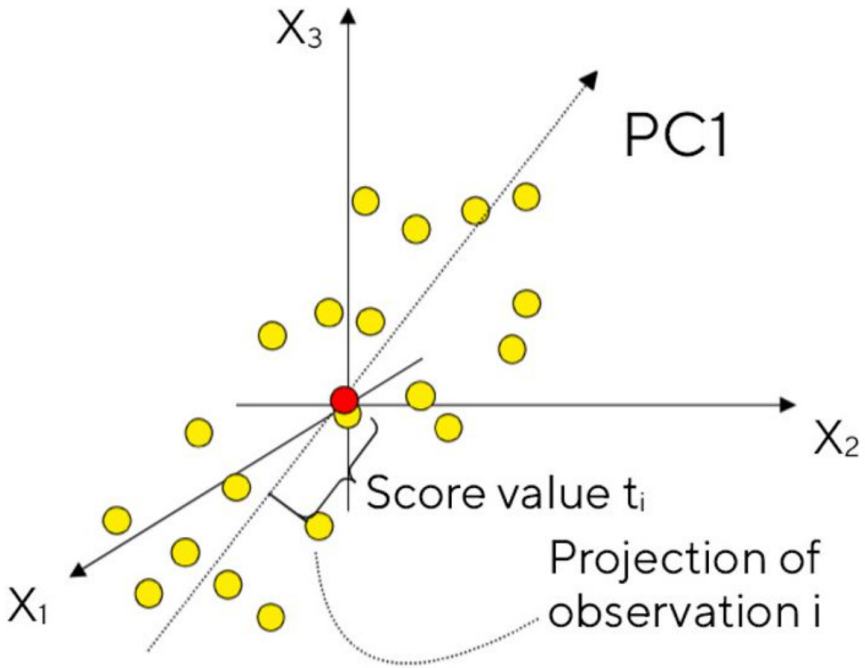

- The first principal component (PC1) is the line that best accounts for the shape of the point swarm. It represents the *maximum variance direction* in the data.

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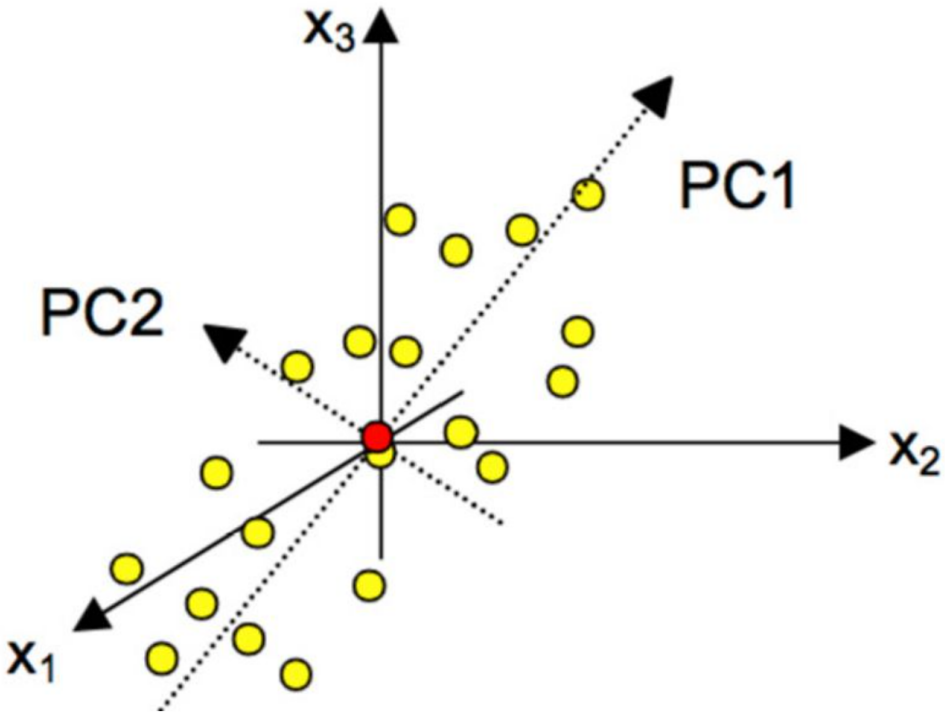

- The second principal component (PC2) is oriented such that it reflects the second largest source of variation in the data while being *orthogonal* to the first PC. PC2 also passes through the average point.

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

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

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

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

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

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

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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.

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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.

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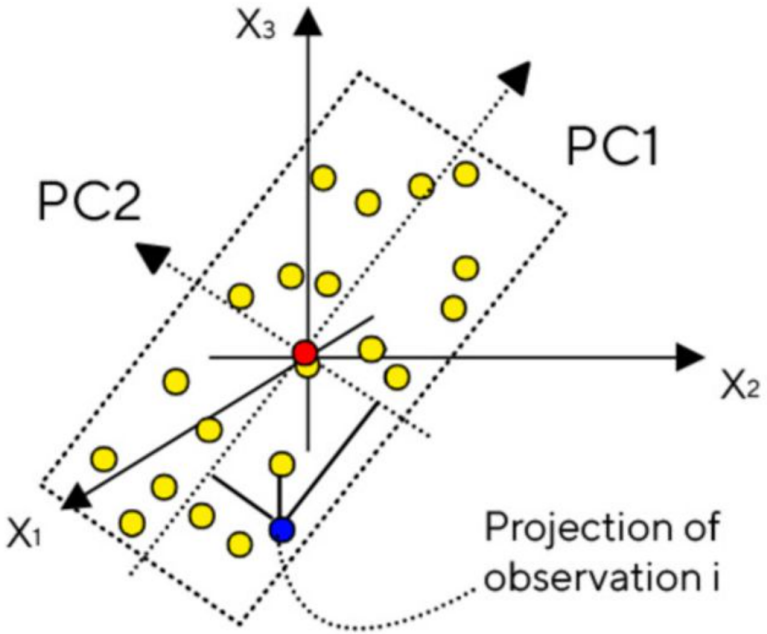

- Two PCs form a plane. This plane is a window into the multidimensional space, which can be visualized graphically. Each observation may be projected onto this plane, giving a **score** for each.

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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

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- The score plot is a map of 16 countries. Countries close to each other have similar food consumption profiles, whereas those far from each other are dissimilar.

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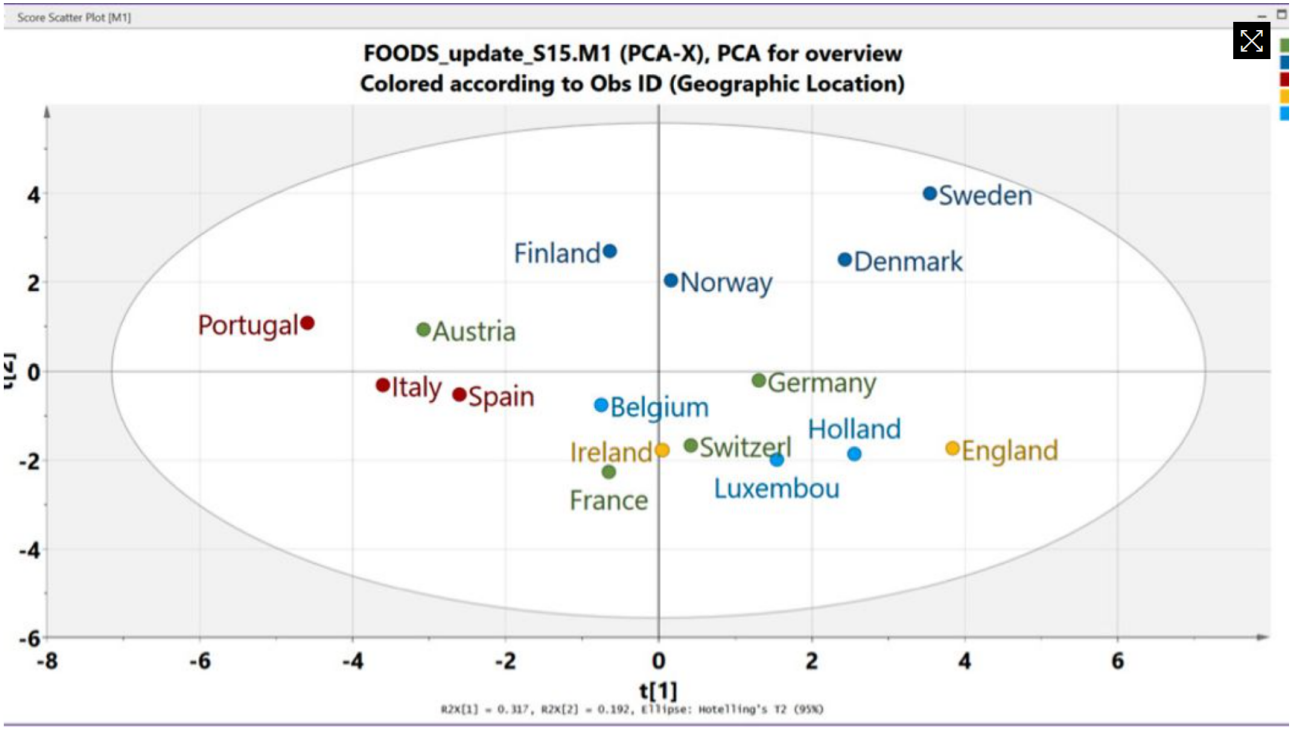

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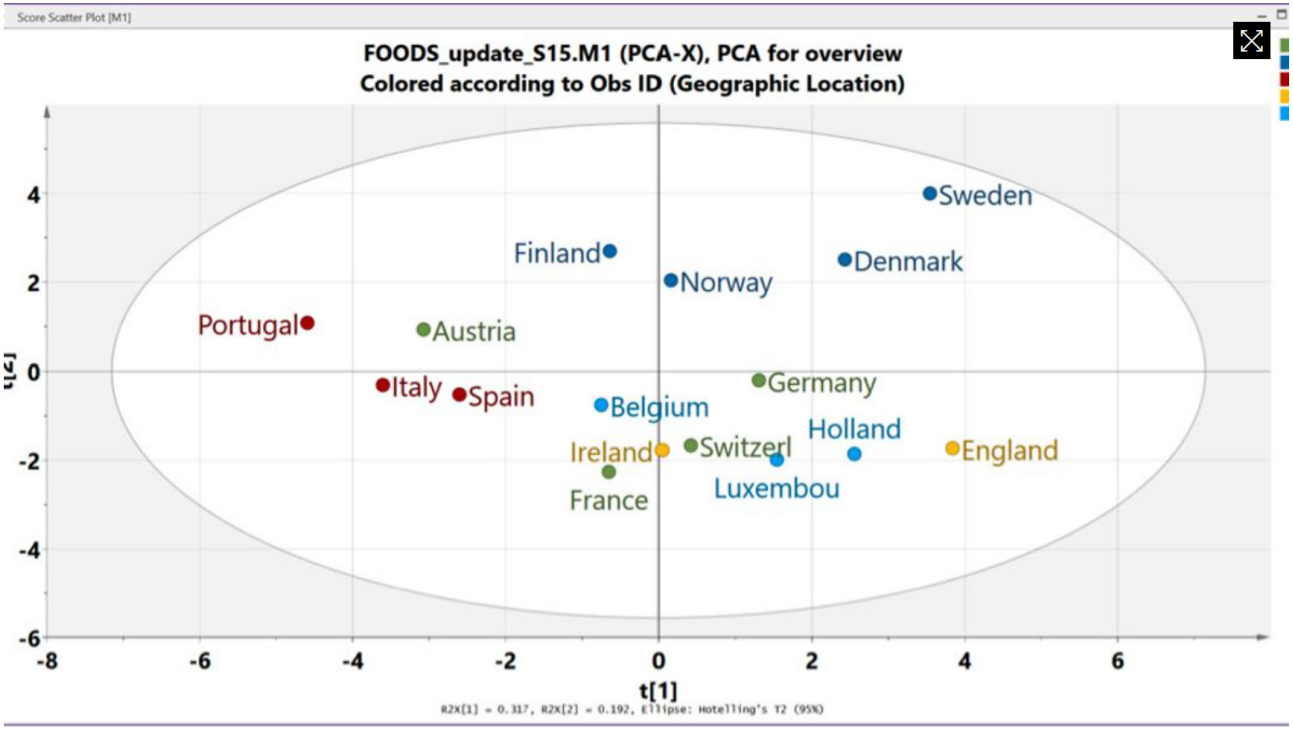

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- The first component explains 32% of the variation, and the second component 19%.

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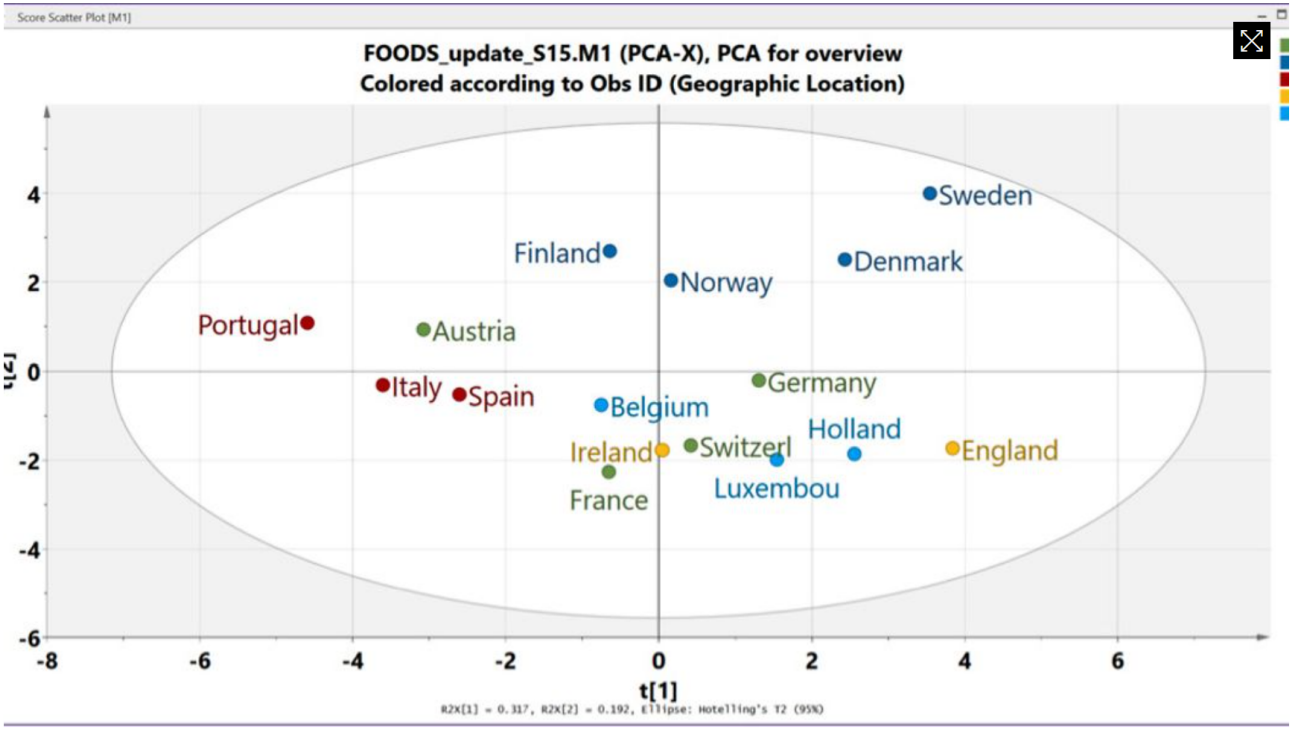

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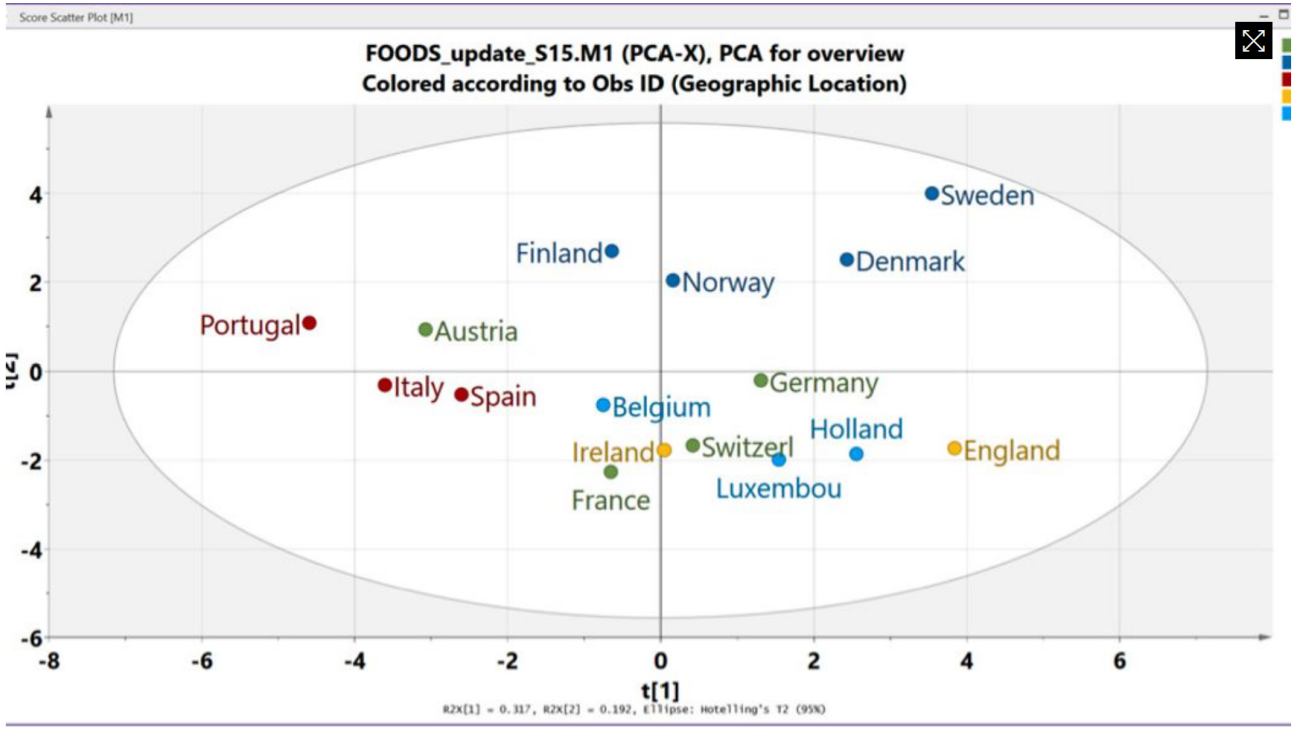

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- Belgium and Germany are close to the center (origin) of the plot, which indicates they have average properties.

Exercise: PCA

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

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

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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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where $||L||_*$ is the trace norm of L, $||S||_1$ is the L_1 norm of S, and λ is a regularization parameter.

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- The trace norm of a matrix A is defined as the sum of its singular values (eigenvalues).
- 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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- Now, the bank can potentially have millions of customers. Does it make sense to look at the details of each customer separately and then make a decision?
- Certainly not! It is a manual process and will take a huge amount of time.

Clustering

- First, let us see an example below:
- A bank wants to give credit card offers to its customers. Currently, they look at the details of each customer and, based on this information, decide which offer should be given to which customer.
- Now, the bank can potentially have millions of customers. Does it make sense to look at the details of each customer separately and then make a decision?
- Certainly not! It is a manual process and will take a huge amount of time.
- So what can the bank do?

Clustering

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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 lable, 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).

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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:

K-Means

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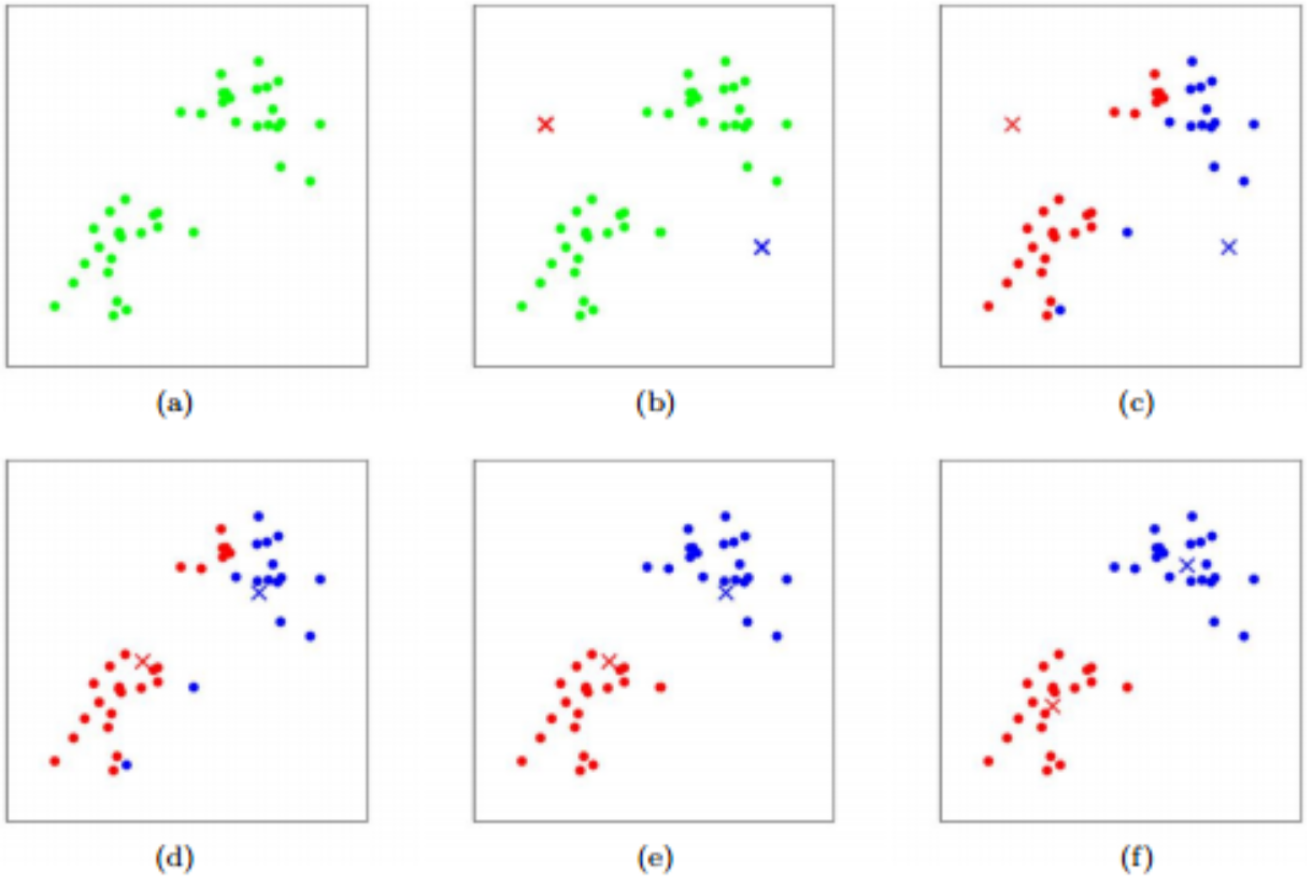
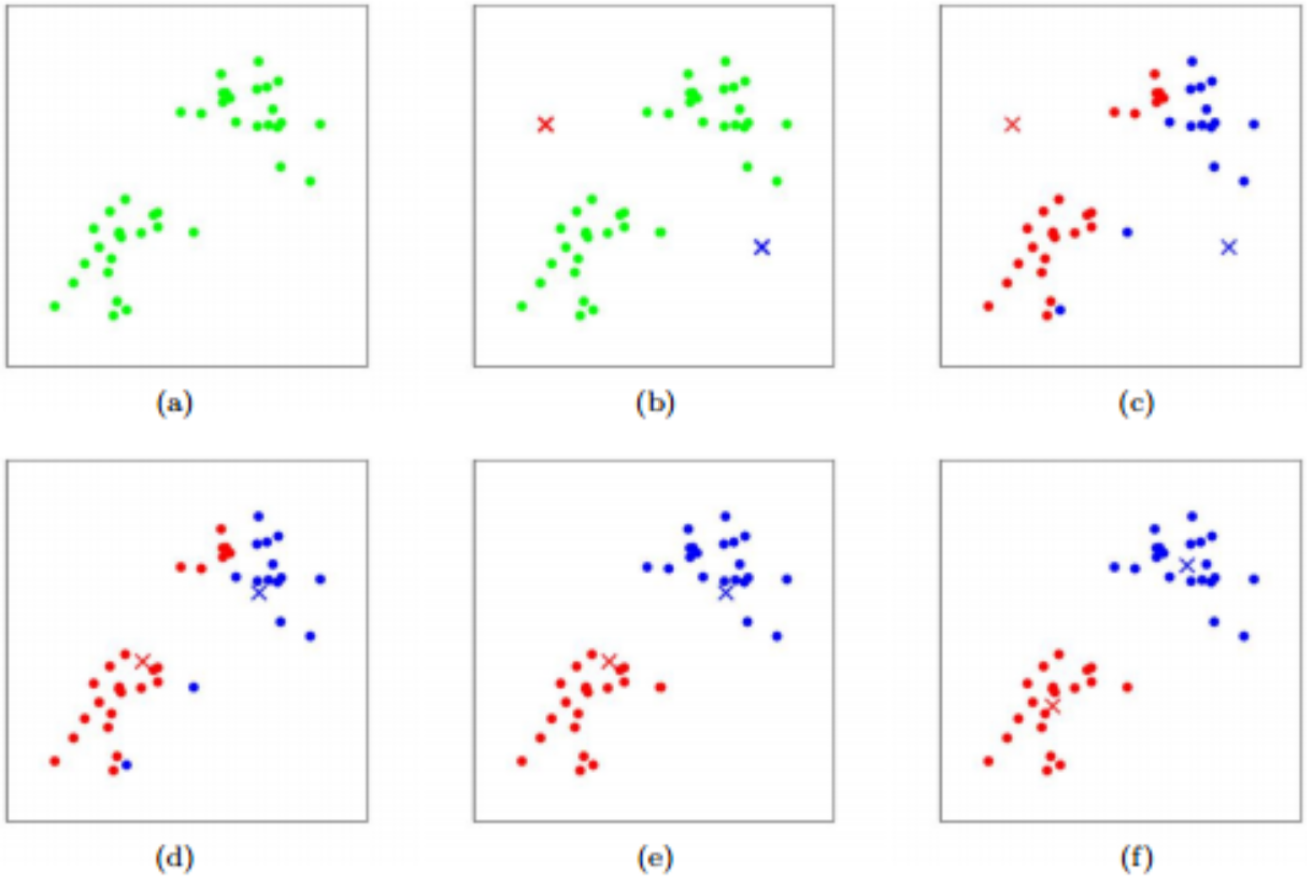
- The value of K is often pre-specififed.

K-Means



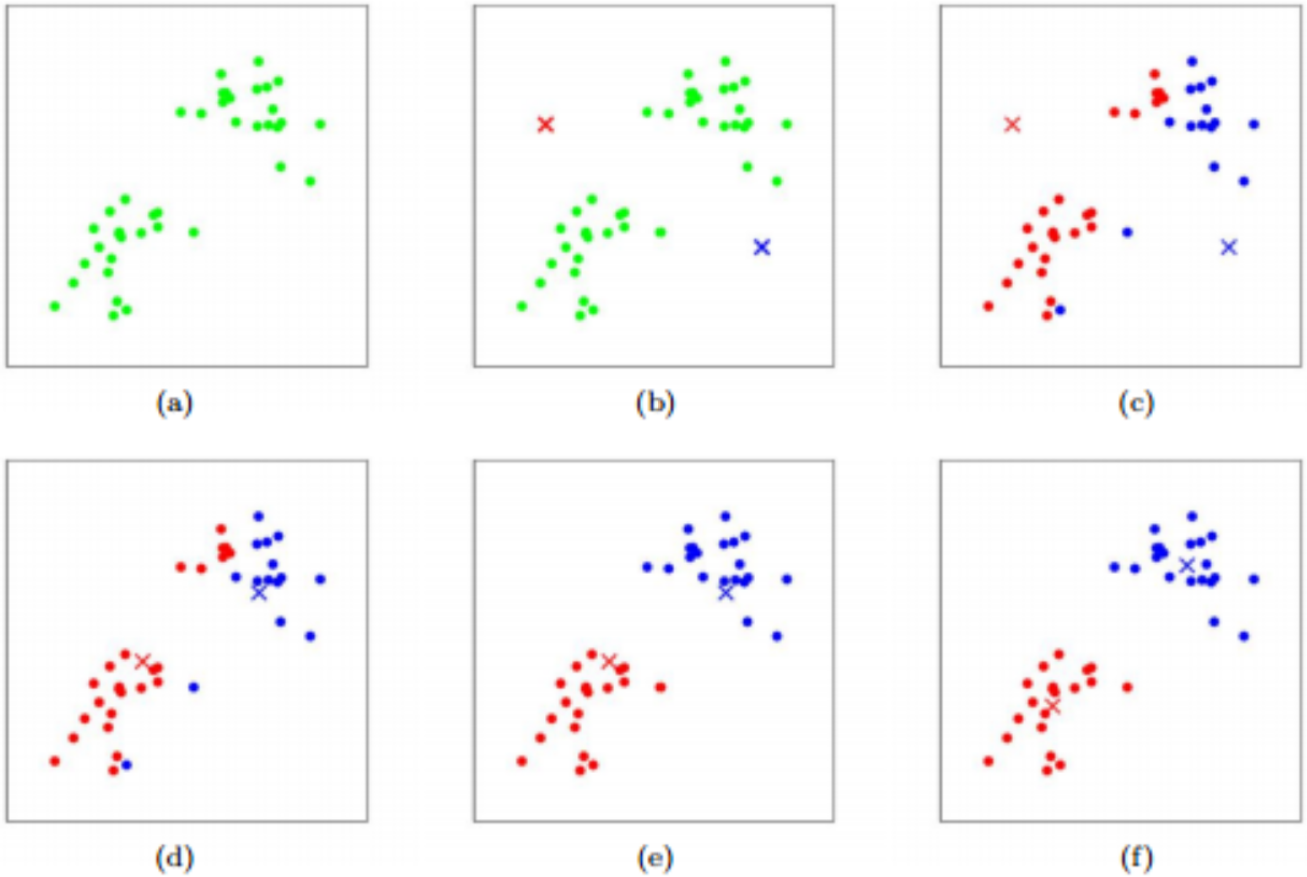
- Training examples are shown as dots, and cluster centroids are shown as crosses.

K-Means



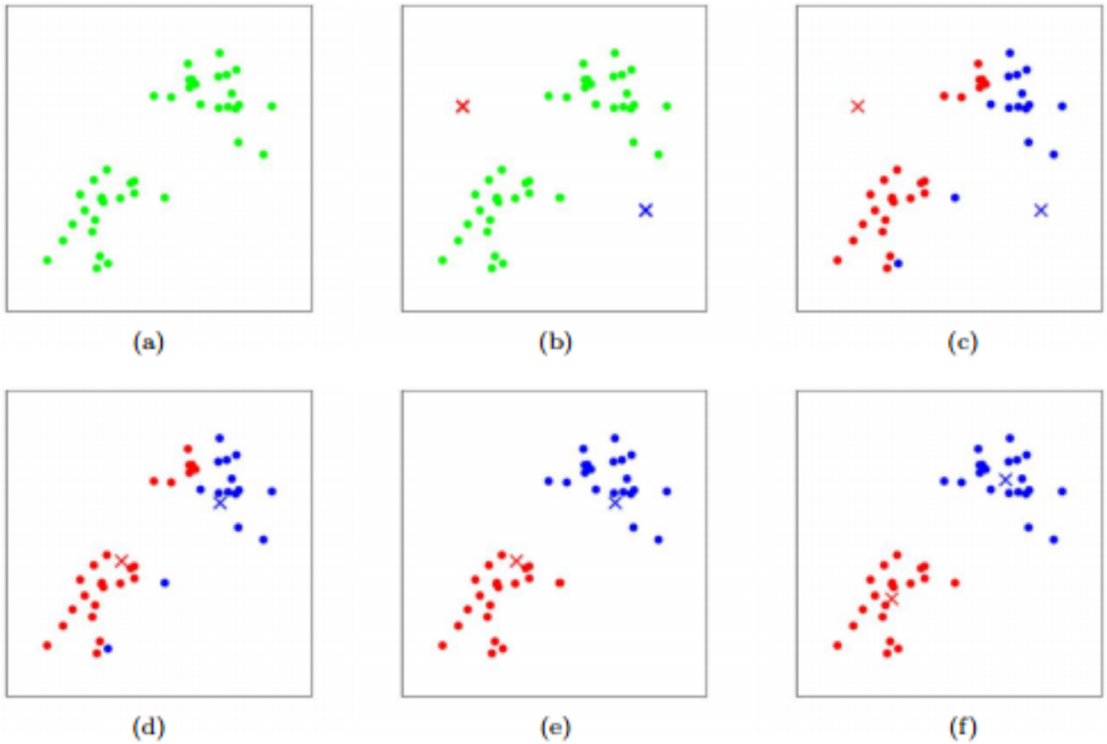
- (a) Original dataset.

K-Means



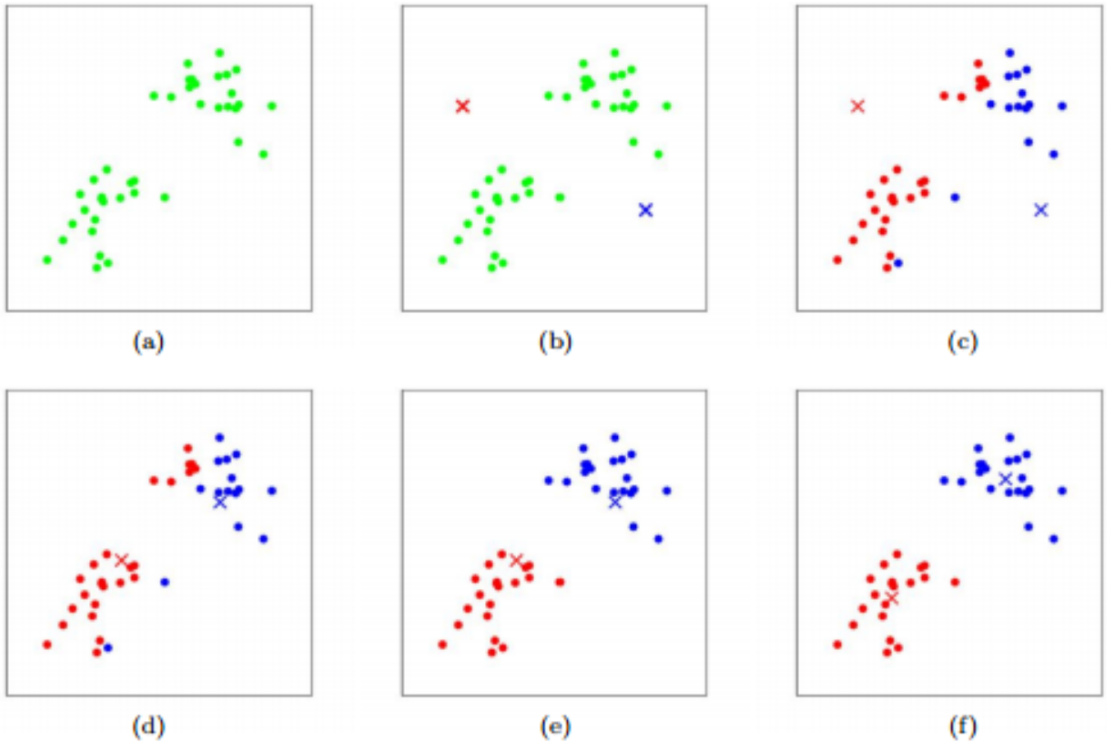
- (b) Random initial cluster centroids.

K-Means



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

K-Means



- In each iteration, we assign each training example to the closest cluster centroid (shown by "painting" the training examples the same color as the cluster centroid to which is assigned);

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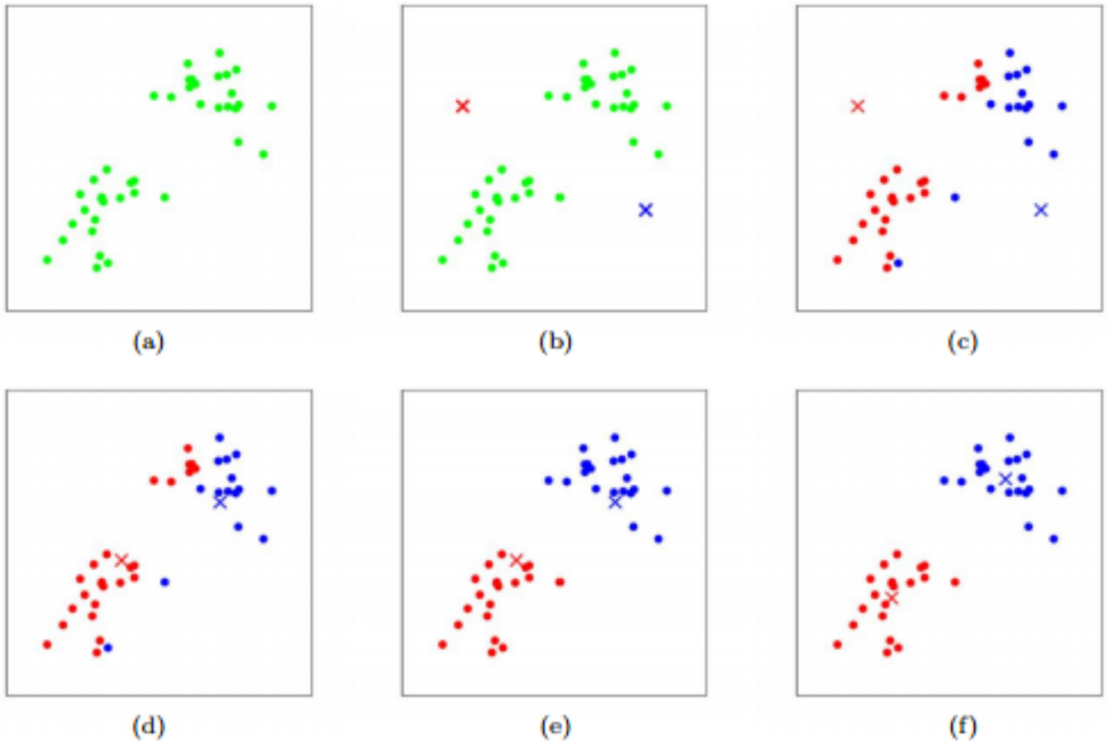

- In each iteration, we assign each training example to the closest cluster centroid (shown by "painting" the training examples the same color as the cluster centroid to which is assigned);
- Then we move each cluster centroid to the mean of the points assigned to it.

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  - For each j, set $\mu_j = \frac{\sum_{i=1}^{m} 1\{c^{(i)}=j\} x^{(i)}}{\sum_{i=1}^{m} 1\{c^{(i)}=j\}}$

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  - (3) Update Centroids: Recalculate the centroids as the mean of the points in each cluster.
  - (4) Repeat Steps 2 and 3 until the centroids do not change.

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- Number of Iterations: 2.

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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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- Given a dataset $X = \{x_1, x_2, \cdots, x_n\}$ consisting of n data points, the the goal of FCM is to partition the data into c fuzzy clusters, where c is a predefined number of 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

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- $||x_i - v_j||$ is the Euclidean distance between the data point x_i and the cluster centerv_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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  - 1) Gives best result for overlapped data set and comparatively better then 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 then one cluster center.

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  - 2) Euclidean distance measures can unequally weight underlying factors.