Econ 425 Week 9

Clustering and PCA

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Motivation

- what if a dataset has too many variables?
- e.g., most of the variables are correlated on analysis
- may lead to poor accuracy in estimation
- **dimension reduction** methods
    - Principal Component Analysis (PCA)

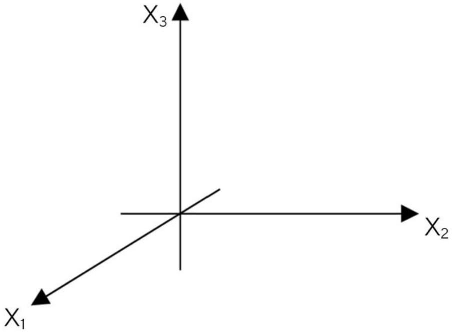
PCA

- summarizes the information content in large datasets with a smaller dataset of “summary indices” that can be more easily visualized and analyzed
- underlying data can be measurements describing properties of production samples, chemical compounds or reactions, time points of a continuous process, batches from a batch process, biological individuals, or trials of a DOE protocol
- often used in the preliminary data analysis, before running any ML tasks

How PCA works

- X is data matrix with N rows (observations) and K columns (features)
- construct a variable space with as many dimensions as there are variables (see figure on the next slide)
- each variable represents a coordinate axis; for each variable, the length is standardized, typically by scaling to unit variance

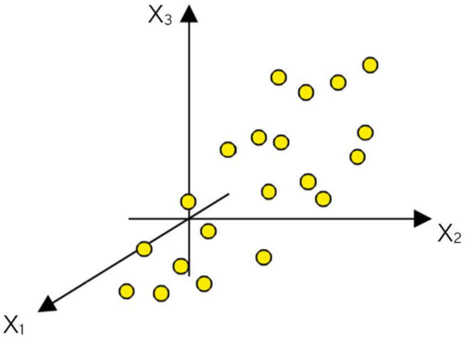
How PCA works



Feature space $\mathbb{R}^K$. Only three variable axes displayed. The "length" of each coordinate is standardized

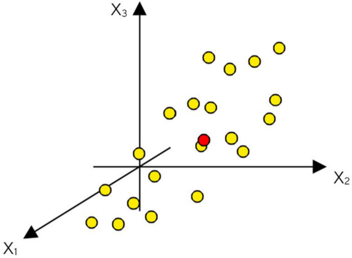
How PCA works

- each observation in X is a point in the feature space $\mathbb{R}^K$



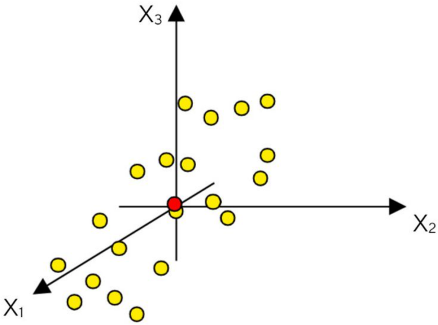
How PCA works

- **centering**: subtract variable averages from the data. The vector of averages is the red point in $\mathbb{R}^K$



How PCA works

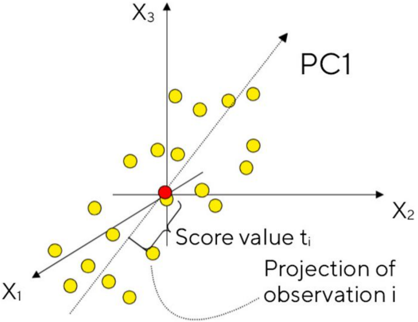
- subtraction of the average corresponds to a re-positioning of the origin of the coordinate system to the average point



How PCA works: first principal component

- ready to compute the first principal component (PC1)
- PC1 is the line through the average point that best approximates the data in the least squares sense
- each observation (yellow dot) may now be projected onto this line to get the coordinate value along the PC-line (**score**)

How PCA works: first principal component

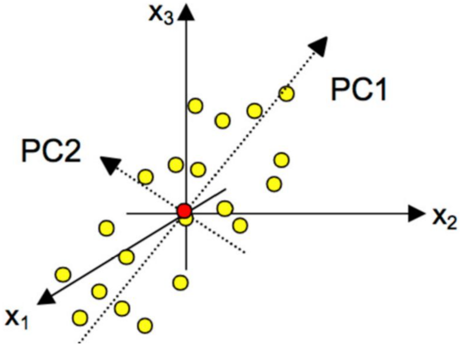


- the first principal component (PC1) represents the *maximum variance direction* in the data

How PCA works: second principal component

- usually one summary index or principal component is insufficient to model the systematic variation of data
- second principal component (PC2) is represented by a line through the average point *orthogonal* to the first PC

The second principal component



- second principal component (PC2) 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 PC1 and PC2?

- **standardize the data**: each variable should be mean 0 and SD 1 (PCA is sensitive to scaling)
- **calculate the sample covariance matrix**

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

  - elements are covariances between each pair of features

How to calculate PC1 and PC2?

- **calculate the eigenvalues and eigenvectors of the covariance matrix**: eigenvectors/eigenvalues represent directions of maximum variance / magnitude of variance in the data
- eigenvectors $\{v_1, v_2, .., v_K\}$ and eigenvalues $\{\lambda_1, \lambda_2, ..\lambda_K\}$ satisfy

$$\widehat{\Sigma} v_k = \lambda_k v_k$$

- eigendecomposition:

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

where V is a matrix of eigenvectors, Λ is a diagonal matrix with eigenvalues on the diagonal

How to calculate the PC1 and PC2 ?

- **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:

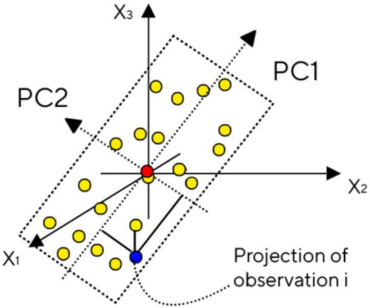
$$PC1 = v_1$$

$$PC2 = v_2$$

The model plane

- PC1 and PC2 together define a plane in $\mathbb{R}^K$
- visualize the data by projecting observations onto this low-dimensional subspace and plotting (**score plot**)
- coordinate values of the observations on this plane **scores**

The model plane



- PC1 and PC2 form a plane, which can be visualized graphically. Projections of observations onto the plane are called **scores**

What is the score?

- PC scores of (standardized) X are obtained by multiplying X by the loadings (eigenvectors) of the covariance of X, say $\widehat{\Sigma}$
- recall that V is the matrix of eigenvectors (loadings) of $\widehat{\Sigma}$
- order the columns of V by their corresponding eigenvalues in descending order
- scores:

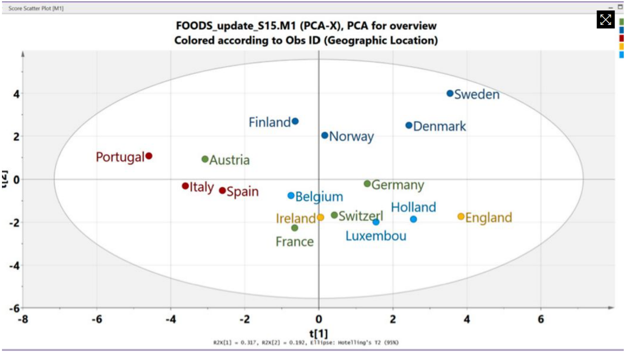
$$T_{n \times k} = XV$$

- the first column of T contains the scores for PC1, the second column contains the scores for PC2, etc.

PCA: example

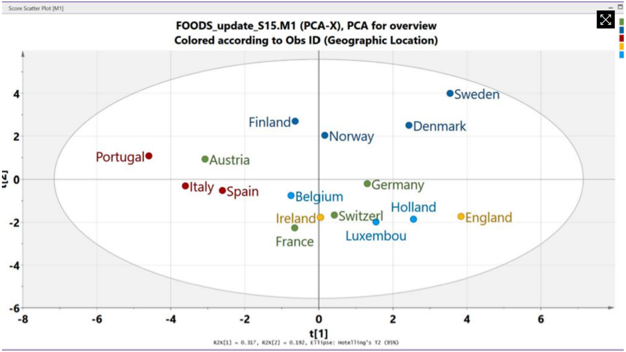
- data: food consumption in European countries
- figure on the next slide displays the score plot of the first two principal components (scores t_1 and t_2)
- the score plot is a map of 16 countries: those close to each other have similar food consumption profiles

PCA: example



- score plot illustrates relations between food consumption profiles
- PC1 (PC2) explains 32% (19%) of the variation of the data

PCA: example



- Nordic countries (Finland, Norway, Denmark, and Sweden) are in the upper right corner
- Belgium and Germany are close to the center (origin) of the plot

PCA: exercise

- dataset:

x_1	x_2
1	2
3	4
5	6

- perform PCA on this dataset by following these steps:
- **demean the data**: subtract the mean of each variable from the corresponding values
- **calculate the covariance matrix** of the centered data
- **find the eigenvalues and eigenvectors** of the covariance matrix
- **choose the principal component(s)**: select the eigenvector(s) associated with the largest eigenvalue(s) as PCs
- **calculate the scores**: project the centered data onto PCs

Exercise: PCA

- demeaned data:

x_1	x_2
-2	-2
0	0
2	2

- covariance matrix:

$$\begin{pmatrix} 4 & 4 \\ 4 & 4 \end{pmatrix}$$

- eigenvalues and eigenvectors:
  - eigenvalues: $0, 8$
  - eigenvectors:

$$\begin{pmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$

$$\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$

PCA: exercise

- choose the principal component(s): eigenvector associated with the largest eigenvalue (8) is $\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$ (PC1)
- calculate the scores (projections of the centered data onto PC1):

  scores = centered data $\times$ PC $= \begin{pmatrix} -2\sqrt{2} & 2\sqrt{2} \\ 0 & 0 \\ 2\sqrt{2} & -2\sqrt{2} \end{pmatrix}$

Shortcomings of standard PCA

- sensitive to outliers and noise, which can significantly affect the computed PCs
- **robust PCA** is designed to separate the low-rank structure of the data (true signal) from the sparse noise or outliers
  - more suitable for datasets corrupted by noise or anomalies

Robust PCA

- objective: decompose X into a low-rank matrix L and a sparse matrix S such that $X = L + S$
- achieved by solving

$$\min_{L,S} \ \ ||L||_* + \lambda ||S||_1$$

$$\text{s.t.} \ \ X = L + S$$

  where $||L||_*$ is the trace norm of L, $||S||_1$ is the L_1 norm of S, and λ is a regularization parameter
- $||L||_*$ is the sum of singular values (eigenvalues of $L'L$)
- $||S||_1$ is the sum of absolute values of entries of S

Clustering

- a bank wants to give credit card offers to its customers; currently, they use customer data to decide which offer should be given to which customer
- the bank can potentially have millions of customers; should it use customer-level data?
- what can the bank do?

Clustering

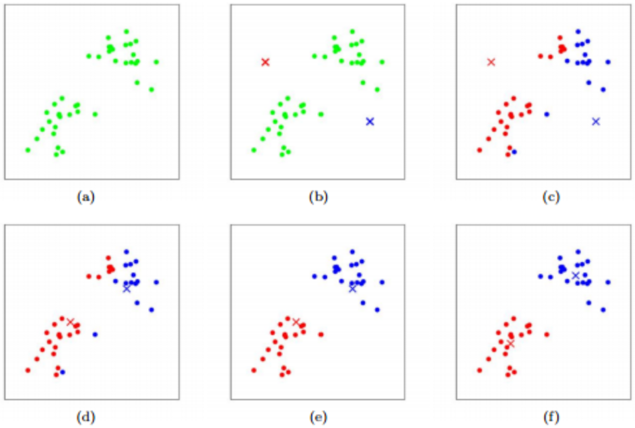
- segment the customers into different groups, e.g. income groups:

- now only three strategies are required, one for each income group
- "high", "average", "low" are not prespecified labels, but outcomes of clustering (**unsupervised learning**)

K-means clustering

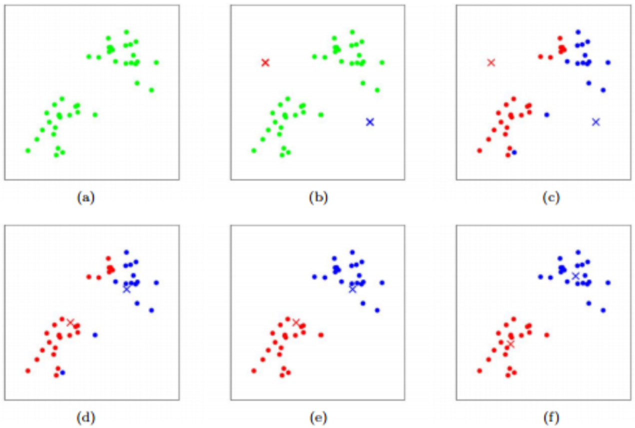
- one of the most popular clustering algorithms
- stores K centroids used to define clusters
- a point is in a cluster if it is closer to that cluster's centroid than any other centroid
- finds the best centroids by alternating between
  1. assigning data points to clusters based on current centroids
  2. choosing centroids based on the current assignment of data points to clusters
- K is either prespecified or tuned, e.g., by cross-validation

K-Means



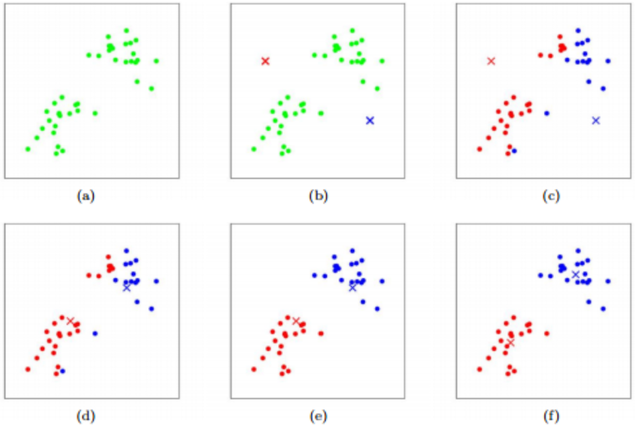
- training examples are dots, cluster centroids are crosses

K-Means



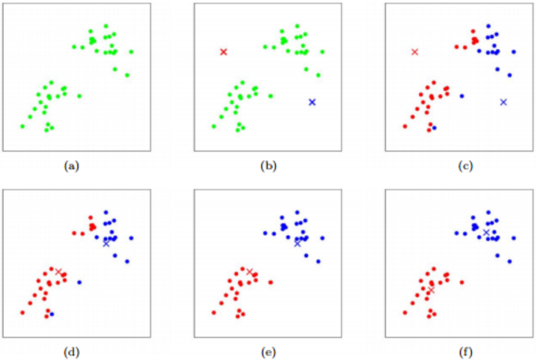
(a) original data

K-Means



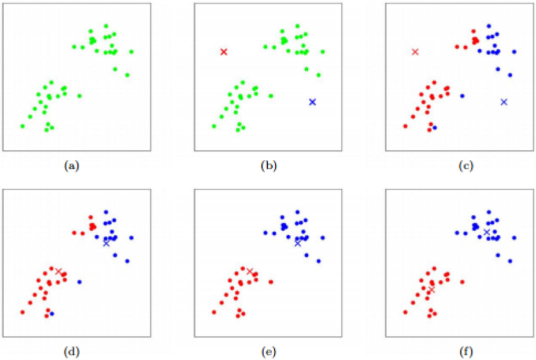
(b) random initialization of cluster centroids

K-Means



(c)-(f) two iterations of K-means clustering

K-Means



- in each iteration, training example are assigned to the closest cluster centroid (shown by coloring the training examples with the same color as the cluster centroid to which is assigned)
- then each cluster centroid is moved to the mean of the points assigned to it

K-Means algorithm

- initialize cluster centroids $\mu_1, \mu_2, \cdots, \mu_K \in \mathbb{R}^d$ randomly
- until convergence, repeat:
    - for each i, set **membership**

$$c^{(i)} = \mathrm{argmin}_j \|x^{(i)} - \mu_j\|^2$$

    - for each j, set **centroids**

$$\mu_j = \frac{\sum_{i=1}^{m} 1\{c^{(i)} = j\} x^{(i)}}{\sum_{i=1}^{m} 1\{c^{(i)} = j\}}$$

Exercise: K-Means on a small dataset

- objective: apply K-Means clustering to a small dataset
- data:
  $X = [(1,1),(1,2),(2,1),(2,2),(4,4),(4,5),(5,4),(5,5)]$
- steps:
  1. initialize centroids: choose $k = 2$ and initial centroids as $(1,1)$ and $(1,2)$
  2. assign points to clusters: assign each point to the nearest centroid
  3. update centroids: recalculate the centroids as the mean of the points in each cluster
  4. repeat steps 2 and 3 until convergence

Exercise: K-Means on a small dataset

- initial centroids:
  - centroid 1: $(1, 1)$
  - centroid 2: $(1, 2)$
- iteration 1:
  - cluster 1: $[(1, 1), (1, 2), (2, 1), (2, 2)]$
  - cluster 2: $[(4, 4), (4, 5), (5, 4), (5, 5)]$
  - new centroids: centroid 1: $(1.5, 1.5)$, centroid 2: $(4.5, 4.5)$
- iteration 2:
  - no change in cluster assignment
  - convergence achieved
- final centroids:
  - centroid 1: $(1.5, 1.5)$
  - centroid 2: $(4.5, 4.5)$
- number of iterations: 2

Fuzzy C-Means clustering

- K means: each observation only belongs to one cluster
- fuzzy C-means: each observation may belong to two or more clusters
  - degree of **membership** of x_i in cluster c
- often used in pattern recognition and is an extension of the traditional K-means clustering

Fuzzy C-Means clustering

- given a dataset $X = \{x_1, x_2, \cdots, x_n\}$, FCM partitions the data into C fuzzy clusters
- each data point x_i has a degree of membership $u_{ic} \in [0, 1]$ in each cluster c

Fuzzy C-Means clustering

FCM objective function:

$$J(U,V) = \sum_{i=1}^{n}\sum_{c=1}^{C} u_{ic}^{m}\|x_i - v_c\|^2,$$

where

- $U = [u_{ic}]$ is the membership matrix
- $V = \{v_1, v_2, \cdots, v_C\}$ are cluster centers
- m is a parameter that controls the level of cluster fuzziness
- $\|x_i - v_c\|$ is the Euclidean distance between the data point x_i and the cluster center v_c

Fuzzy C-Means clustering

- iteratively updates membership matrix U and cluster centers V until convergence
- **membership** update:

$$u_{ic}^m = \frac{1}{\sum_{k=1}^{C} \left(\frac{\|x_i - v_c\|}{\|x_i - v_k\|}\right)^{\frac{2}{m-1}}}$$

- **cluster center** update:

$$v_c = \frac{\sum_{i=1}^{n} u_{ic}^m x_i}{\sum_{i=1}^{n} u_{ic}^m}$$

- stops when changes in membership matrix between consecutive iterations are below a specified threshold

Fuzzy C-Means: example

- dataset with four points: A, B, C, and D
- cluster these points into $C = 2$ clusters using Fuzzy C-means
- membership values:

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

Fuzzy C-Means: example

- **point A** has a high membership value (0.8) in cluster 1 and a low membership value (0.2) in cluster 2, i.e. point A is strongly associated with Cluster 1 but has a slight association with Cluster 2
- **point B** has a membership value of 0.3 in cluster 1 and 0.7 in cluster 2, indicating that it is more closely associated with Cluster 2
- **point C** has a membership value of 0.6 in cluster 1 and 0.4 in cluster 2, suggesting that it belongs more to Cluster 1 but still has some association with Cluster 2
- **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

Fuzzy C-Means clustering

Advantages:

- good for overlapping data
- fuzzy membership

Disadvantages:

- number of clusters should pre-specified
- Euclidean distance may unequally weight underlying factors