# Software Development for Data Analysis

# Principal Component Analysis (PCA)

- A statistical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables called principal components.
- The analyzed data consist in a table of observations, having ***n*** rows and ***m*** columns.

$$X = \begin{bmatrix} x_{11} & \cdots & x_{1m} \\ \cdots & & \\ x_{n1} & .. & x_{nm} \end{bmatrix}$$

, where $x_{ij}$ is the value taken by variable $j$ for the observation $i$.

- The variable described by table X are also known as *initial*, *causal or observed variables*.

# Principal Component Analysis (PCA)

- $\boldsymbol{X_j}$ is the column vector containing the values of variable $\boldsymbol{j}$ for $\boldsymbol{n}$ observations;
- The goal of the procedure is to describe table $X$ through a reduced number of nonrelated variables: $C_1$, $C_2$, ..., $C_s$.

**Phase 1**

Determine a new variable $C_1$, the first principal component, as linear combination of variables $X_j$:

$$C_1 = a_{11}X_1 + ... + a_{j1}X_j + ... + a_{m1}X_m$$

The value taken by $C_1$ for a given observation $i$ :

$$c_{i1} = a_{11}x_{i1} + ... + a_{j1}x_{ij} + ... + a_{m1}x_{im}$$

where $a_{j1},\ j = \overline{1,m}$

# Principal Component Analysis (PCA)

**Phase k**

Determine a new variable $C_k$, the k principal component, as linear combination of variables $X$:

$$C_k = a_{1k} X_1 + ... + a_{jk} X_j + ... + a_{mk} X_m \quad ,$$

where $a_k$ is the vector containing the multipliers $a_{jk}, j = \overline{1, m}$

The link between the causal variables ($X$) and the principal components ($C$) is given by:

$C_k = X \cdot a_k$, $k=1,s$ , where $\boldsymbol{s}$ is the number of principal components.

# Principal Component Analysis (PCA)

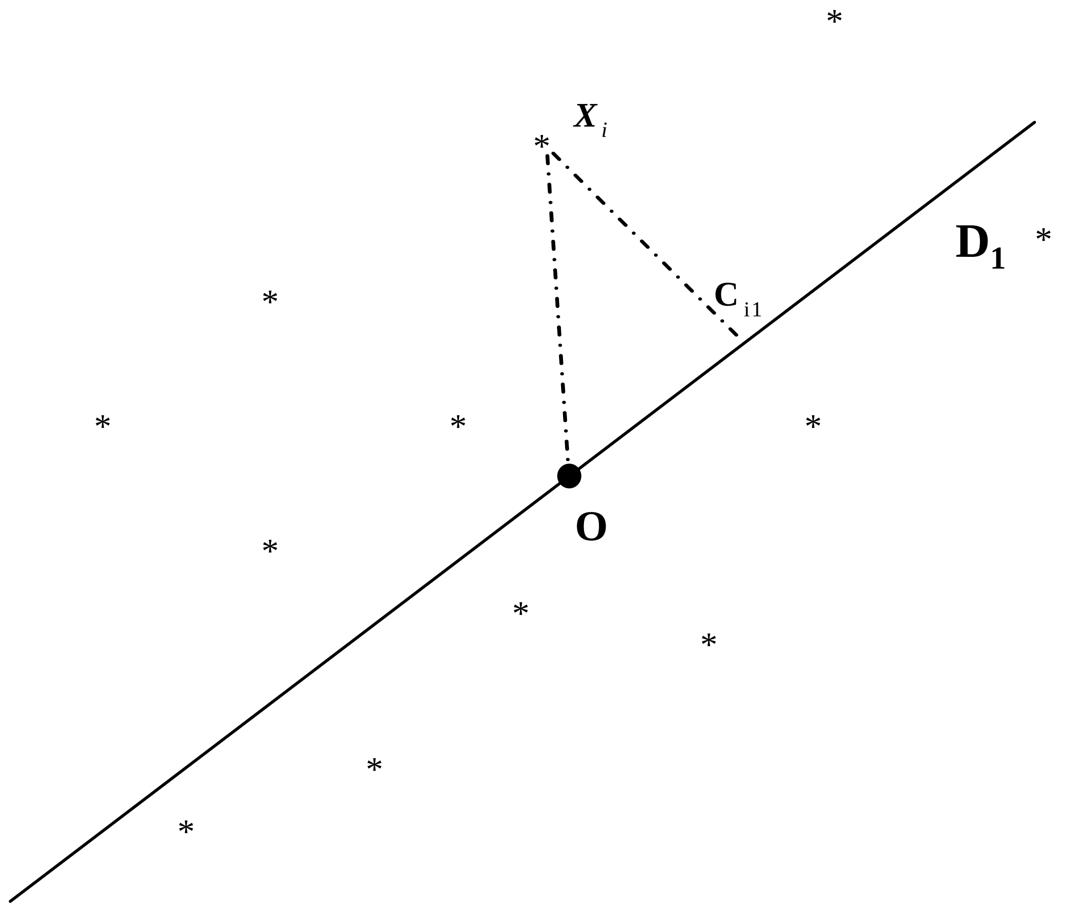
**Observation driven approach**

- The cloud of observations has ***n*** points within a ***m***-dimensional space;
- Those ***m*** variables determine the ***m*** axis of coordinates;
- If the data is standardized, then the variables have the mean 0, and the standard deviation 1;
- Consider a system of orthonormal axes (it is orthogonal and having the norm 1) for those ***n*** points;
- Each axis corresponds to one principal component, and the vectors $a_k$ are unit vectors (in a normed vector space, it is a vector, often a spatial vector, of length 1):

$$\sum_{j=1}^{m} {a_{kj}}^{2} = 1, k = \overline{1, s}$$ , where ***s*** is the maximum number of axes

# Principal Component Analysis (PCA)

**Observation driven approach: projection on $D_1$ axis**



# Principal Component Analysis (PCA)

**Observation driven approach**

**Step 1**

- Determine first axis, corresponding to the first principal component, so the component's variance is maxim;
- **O** is the center of gravity for the cloud of points;
- The distance from the point (observation) $X_i$ to the $D_1$ axis, corresponding to the first principal component is $d(i, D_1)$;
- The distance from $X_i$ to origin **O** is $d(i, \mathbf{O})$.

Then we have the following relation between distances in the corresponding right-triangle:

$d(i, \mathbf{O})^2 = d(i, D_1)^2 + c_{i1}^2$, where $c_{i1}$ is the projection of $X_i$ on $D_1$ axis.

# Principal Component Analysis (PCA)

**Observation driven approach**

- Therefore, for all the points in the cloud we have the following equality of sums:

$$\frac{1}{n}\sum_{i=1}^{n} d(i,O)^2 = \frac{1}{n}\sum_{i=1}^{n} d(i,D_1)^2 + \frac{1}{n}\sum_{i=1}^{n} c_{i1}^2$$

# Principal Component Analysis (PCA)

**Observation driven approach**

- The sum of the distances toward the center of gravity (*barycenter*) does not depend on the chosen axis;
- The *variance explained through axis 1* is $\frac{1}{n}\sum_{i=1}^{n} c_{i1}^{2}$
- Which in terms of matrixes, knowing that $(Xa)^t = a^t X^t$, we then have:

  $C_1 = X \cdot a_1$ , then square the equality and divede by *n* (no. of observations)

$$\frac{1}{n}(C_1)^t C_1 = \frac{1}{n}(a_1)^t X^t X a_1$$

The problem is to dually (complementary) reach the same goal:

1. Maximize the explained variance on axis 1;
2. Minimize the sum point distances to axis 1.

# Principal Component Analysis (PCA)

**Observation driven approach**

$$\begin{cases} \underset{a^1}{Max} \dfrac{1}{n}(a_1)^t X^t X a_1 \\ subject\ of\ (a_1)^t a_1 = 1 \end{cases}$$

Lagrange function (or Lagrangean) associated to the problem is defined by:

$$L(a_1, \lambda) = \frac{1}{n}(a_1)^t X^t X a_1 - \lambda((a_1)^t a_1 - 1)$$

where λ is a Lagrange multiplier.

# Principal Component Analysis (PCA)

**Observation driven approach**

**Partial derivatives:**

$$\frac{\partial L}{\partial a_1} = 2\frac{1}{n}X^t X a_1 - 2\lambda a_1 = 0 \qquad \frac{\partial L}{\partial \lambda} = (a_1)^t a_1 - 1 = 0$$

Having then $\frac{1}{n}X^t X a_1 = \lambda a_1$ .

Therefore $a_1$ is a *eigenvector* of the matrix $\frac{1}{n}X^t X$ , corresponding to the *eigenvalue* (*characteristic value*) λ.

Multiplying on the left with $(a_1)^t$ we have:

$$\frac{1}{n}(a_1)^t X^t X a_1 = \lambda$$

# Principal Component Analysis (PCA)

Then

$\frac{1}{n}(a_1)^t X^t X a_1$ is the quantity we need to maximize.

Therefore:

- $\lambda$ is the greatest characteristic value (eigenvalue), and $a_1$ is the corresponding characteristic vector (eigenvector);
- we shall assign $\lambda$ to $\alpha_1$.

# Principal Component Analysis (PCA)

**Step 2**

- Determine axis 2 described by vector $a_2$ so axis 2 is orthogonal with axis 1;
- Maximize the explained variance (the points are more scattered, disperse on the axis);
- The applied optimization is:

$$\begin{cases} \underset{a_2}{Max} \dfrac{1}{n}(a_2)^t X^t X a_2 \\ (a_2)^t a_2 = 1 \\ (a_2)^t a_1 = 0 \end{cases}$$

$$L(a_2, \lambda_1, \lambda_2) = \frac{1}{n}(a_2)^t X^t X a_2 - \lambda_1((a_2)^t a_2 - 1) - \lambda_2 (a_2)^t a_1$$

# Principal Component Analysis (PCA)

**Step 2**

Set the partial derivative on $a_2$ to zero:

$$\frac{\partial L}{\partial a_2} = 2\frac{1}{n}X^t X a_2 - 2\lambda_1 a_2 - \lambda_2 a_1 = 0$$

Multiplying on the left with $(a_1)^t$ we obtain:

$$2\frac{1}{n}(a_1)^t X^t X a_2 - 2\lambda_1 (a_1)^t a_2 - \lambda_2 (a_1)^t a_1 = 0$$

# Principal Component Analysis (PCA)

**Step 2**

Then we have: $(a_1)^t a_2 = 0$ , since:

$$\frac{1}{n} X^t X a_1 = \alpha_1 a_1$$ through transposition, it implies that

$$(a_1)^t \frac{1}{n} X^t X = \alpha_1 (a_1)^t$$

since the matrix $X^t X$ is symmetrical. Then, multiplying with 2 and $a_2$ on the right hand side:

$$2\frac{1}{n}(a_1)^t X^t X a_2 = 2\frac{1}{n}\alpha_1 (a_1)^t a_2 = 0$$

Therefore $\lambda_2 = 0.$

# Principal Component Analysis (PCA)

**Step 2**

Making the substitution in the derivative

$$\frac{1}{n} X^t X a_2 = \lambda_1 a_2$$

and therefore $a_2$ is eigenvector corresponding to eigenvalue $\lambda_1$ , and this eigenvalue is maximal having given the equality:

$$\frac{1}{n} (a_2)^t X^t X a_2 = \lambda_1$$

Since $\frac{1}{n} X^t X a_2 = \lambda_1 a_2$ it is maximized at this step, we shall assign $\lambda_1$ to $\alpha_2$

# Principal Component Analysis (PCA)

**Step *k***

- Determine $k$ axis of $a_k$ vector, orthogonal on the previous axis and to maximize the explained variance;
- The optimum problem is as follows:

$$\begin{cases} \underset{a^k}{Max} \dfrac{1}{n} (a_k)^t X^t X a_k \\ (a_k)^t a_k = 1 \\ (a_k)^t a_j = 0,\ j = \overline{1, k-1} \end{cases}$$

# Principal Component Analysis (PCA)

**Step *k***

The associated Lagrange function L($a_k$, $\lambda_1$, $\lambda_2$,..., $\lambda_k$) is as follows:

$$L(a_k, \lambda_1, \lambda_2, \ldots, \lambda_k) = \frac{1}{n}(a_k) X^t X a_k - \lambda_1((a_k)^t a_k - 1) - \lambda_2 (a_k)^t a_1 - \ldots - \lambda_k (a_k)^t a_{k-1}$$

Setting the derivative on zero:

$$\frac{\partial L}{\partial a_k} = 2\frac{1}{n} X^t X a_k - 2\lambda_1 a_k - \lambda_2 a_1 - \ldots - \lambda_k a_{k-1} = 0$$

Then multiply the first relation successively with $(a_1)^t$, $(a_2)^t$,..., $(a_{k-1})^t$, and obtain $\lambda_2 = 0$ , $\lambda_3 = 0$, ..., $\lambda_k = 0$. Returning with these results to the first partial derivative we have:

$$\frac{1}{n} X^t X a_k = \lambda_1 a_k$$

# Principal Component Analysis (PCA)

**Step *k***

Therefore $a_k$ is eigenvector of matrix $\frac{1}{n}X^tX$ , corresponding to eigenvalue $\lambda_1$, and since the quantity

$$\frac{1}{n}(a_k)^t X^t X a_k$$

it is the one maximized at this step, then $\lambda_1$ is eigenvalue of *k* order.

We shall assign $\lambda_1$ to $\alpha_k$.

# Principal Component Analysis (PCA)

**PCA in variable spaces**

**Phase 1**

Determine the first principal component $C_1$ so it is maximally correlated with initial, causal variables:

$$\sum_{j=1}^{m} R^2(C_1, X_j) \quad \text{to be maxim}$$

$$R^2(C_1, X_j) = \frac{Cov(C_1, X_j)^2}{Var(C_1)Var(X_j)} = \frac{1}{n}\frac{(C_1)^t X_j (X_j)^t C_1}{(C_1)^t C_1}$$

$$\sum_{j=1}^{m} R^2(C_1, X_j) = \frac{1}{n}\sum_{j=1}^{m}\frac{(C_1)^t X_j (X_j)^t C_1}{(C_1)^t C_1} = \frac{1}{n}\frac{(C_1)^t X X^t C_1}{(C_1)^t C_1}$$

# Principal Component Analysis (PCA)

**PCA in variable spaces**

**Phase 1**

Solve the following problem:

$$\underset{C_1}{Maxim}\frac{1}{n}\frac{(C_1)^t XX^t C_1}{(C_1)^t C_1}$$

The solution is the eigenvector of matrix $\frac{1}{n}XX^t$, corresponding to the greatest eigenvalue $\beta_1$:

$$\frac{1}{n}XX^t \cdot C_1 = \beta_1 \cdot C_1$$

# Principal Component Analysis (PCA)

**PCA in variable spaces**

**Phase 2**

Determine the second principal component $C_2$, maximally correlated with initial variables and not correlated at all with the first principal component $C_1$.

$$\begin{cases} \underset{C^2}{Maxim} \dfrac{1}{n} \dfrac{(C_2)^t XX^t C_2}{(C_2)^t C_2} \\ R(C_1, C_2) = 0 \end{cases}$$

The solution is the eigenvector of the matrix $\frac{1}{n} XX^t$ , corresponding to the second eigenvalue $\beta_2$:

$$\frac{1}{n} XX^t \cdot C_2 = \beta_2 \cdot C_2$$

# Principal Component Analysis (PCA)

**PCA in variable spaces**

**Phase *k***

Determine the principal component $C_k$, maximally correlated with initial variables and not correlated at all with the components previously determined, $C_i$, $i$=1,$k$-1.

$$\begin{cases} \underset{C^1}{Maxim} \dfrac{1}{n} \dfrac{(C_k)^t XX^t C_k}{(C_k)^t C_k} \\ R(C_k, C_i) = 0, i = \overline{1, k-1} \end{cases}$$

The solution is the eigenvector of the matrix $\frac{1}{n} XX^t$, corresponding to the $k$ eigenvalue $\beta_k$:

$$\frac{1}{n} XX^t \cdot C_k = \beta_k \cdot C_k$$

# Principal Component Analysis (PCA)

**The link between the two approaches**

In the observation spaces, at step $k$ it is determined the eigenvector $a_k$, which is the unit vector of $k$ axis, corresponding to $C_k$ component:

$$\frac{1}{n} X^t X \cdot a_k = \alpha_k a_k$$

Multiplying this equation on the left with $X$ we obtain:

$$\frac{1}{n} XX^t X a_k = X \alpha_k a_k \;\; \Rightarrow \;\; \frac{1}{n} XX^t C_k = \alpha_k C_k$$

# Principal Component Analysis (PCA)

**The link between the two approaches**

It is the same equality obtained in the variable spaces approach, if considered $\beta_k = \alpha_k$

$$\frac{1}{n} XX^t C_k = \beta_k C_k$$

The maximum number of steps in the observation spaces may be ***m*** (the rank of matrix $\frac{1}{n} X^t X$ ), while in the variable spaces, the maximum number of steps may be ***n*** (the rank of matrix $\frac{1}{n} XX^t$ ).

The number of non-zero eigenvalues is ***min*****(*****m*****,** ***n*****).**