

## Unit 3.- Principal component analysis (PCA)

Bachelor's Degrees in: Computer Science and Mathematics; Mathematics; Physics and Mathematics  
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Teaching period: 12/09/2023 - 22/12/2023

## 1 Preliminaries

- Objective, usefulness, limitations and prior assumptions
- Principal components

## 2 Formal aspects

- Problem statement
- Problem resolution

## 3 Practices with R language

- PCA Practice 1.1
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## Objective and usefulness

- The **objective** of Principal Component Analysis (PCA) is to **condense the information** provided by multiple variables into a few of them or a few **linear combinations** of them (with **maximum variability**).
- Its **main utility** is as a **preliminary analysis** before applying other statistical techniques such as regression, clustering, etc.

## Limitations

- The main drawback of these methods is the **difficulty in validating the results**.
- It is a **method highly sensitive to outliers** (extreme or atypical values).

## Prior assumptions

- **Correlated variables.**
- **Absence of outliers.**

**Outliers** in any of the variables **require a detailed analysis** as they influence the final outcome of dimensionality reduction.

- **Standardized data** (mean 0 and standard deviation 1).

This prevents variables with a larger scale from dominating the others.

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## What is a principal component?

- **Principal components** are linear combinations of the original variables with maximum variance and are perpendicular to each other.
- In the following section, it will be demonstrated that the **coefficients** of these linear combinations are the **eigenvectors of the covariance matrix**, and their **variances** will be the **associated eigenvalues** of these eigenvectors.
- In other words, PCA **identifies the directions in which the variance is higher**.

## Practical calculation of principal components

- To obtain the **first principal component**, an **optimization problem** is solved to find the weights (loadings) that **maximize the variance**.
- Once the **first component is calculated**, the **second component** is calculated by repeating the same process, but adding the condition that the linear combination cannot be correlated with the first component. This is equivalent to saying they **must be orthogonal**. **The process is iteratively repeated** until all possible components are calculated or until it is decided to stop the process.
- The order of **importance of the components** is determined by the magnitude of the eigenvalue associated with each eigenvector.
- In the next section, it will be justified that one way to solve this optimization problem is by calculating **eigenvectors and eigenvalues** of the covariance matrix.



## Interpretation of the principal components

- The vector defining the **first principal component** follows the **direction in which the observations vary the most**.
- The **second component** follows the direction in which the data exhibit **the highest variance** and is **uncorrelated with the first one** (they are orthogonal directions), and so on for the third and subsequent principal components.

## Proportion of explained variance

- How much of the original information is lost when projecting the observations into a lower-dimensional space? In other words, how much information does each of the obtained principal components capture?

This information is provided by **the proportion of explained variance**, as well as **the cumulative proportion of explained variance**.

- These quantities are very **important** when **deciding on the appropriate number** of principal components.

## Appropriate number of principal components

**There is no single criterion or method** that allows for identifying the optimal number of principal components to use. Different approaches can include:

- **Evaluate the cumulative proportion of explained variance** and select the **minimum number of components beyond which the increase ceases to be substantial**.
- Calculate the **average of the variances explained by each principal component**, and take as many principal components as the number of variances that exceed this average.
- etc.

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## Notations

In this section, a formal justification is provided for how **the principal components are identified with the eigenvectors of the covariance matrix**, as well as **their variances being identified with the associated eigenvalues** of said vector.

Let  $X_1, X_2, \dots, X_p$  be a set of  $p$  **correlated random variables**. Let's denote  $X = (X_1, X_2, \dots, X_p)^t$  the random vector they define. It is assumed  $X$  is **centred**,  $E[X] = 0$ , and let's denote by  $R = E[XX^t]$  its **covariance matrix**.

Let's consider (**no more of  $p$** ) variables defined by:  $U_1 = a_1^t X, \dots, U_q = a_q^t X$ . The objective pursued is to obtain the suitable  $a_1, \dots, a_q \in \mathbb{R}^p, q \leq p$ .

**Prior requirements:**

- $U_1 = a_1^t X, \dots, U_q = a_q^t X$  must be **uncorrelated**. This way, **redundant information will be eliminated**.
- The **variance** of each  $U_i, i \in 1, \dots, q$  is **maximum**. This way, the new variables **will provide meaningful information**.

### Problem statement

Under the aforementioned conditions, the goal is to find  $U_1 = a_1^t X, \dots, U_q = a_q^t X$ , mutually uncorrelated, with each  $U_i$  having maximum variance among all linear combinations of  $X$  that are uncorrelated with  $U_1 = a_1^t X, \dots, U_{i-1} = a_{i-1}^t X$ .

- The variables  $U_1 = a_1^t X, \dots, U_q = a_q^t X$  solution to the previous problem are referred to as the **principal components**.

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## Problem resolution

As previously mentioned, the **resolution of this problem is sequential**:

- First,  $U_1$  is obtained by imposing that it has maximum variance.
- Next,  $U_2$  is **obtained** by imposing that it has the highest variance among all uncorrelated (orthogonal) linear combinations with  $U_1$ .
- The same procedure is followed to **obtain**  $U_3$  by now imposing that it has the highest variance among all linear combinations orthogonal to  $U_1$  and  $U_2$
- For the rest of the principal components **up to**  $U_q$ , **the procedure is the same**.

Next, it will be justified **how the coefficients of the principal components are the eigenvectors of the covariance matrix**, associated with the eigenvalues of largest magnitude at each step.

## Problem resolution - Step 1

In this first step, we obtain the first principal component,  $U_1$ , maximizing its variance. To ensure the existence of this maximum, bounding conditions on the weight vector must be imposed, in this case, that  $a_1$  is a unit vector.

$$\begin{aligned} & \max \text{Var}[U_1] \\ \text{s.a. } & \|a_1\| = a_1^t a_1 = 1 \end{aligned}$$

Considering that  $X$  is a centred random vector,  $E[X] = 0$ , then  $E[a_1^t X] = 0$ , which implies that:

$$\text{Var}[U_1] = E[U_1^2] = E[a_1^t X a_1^t X] = E[a_1^t X X^t a_1] = a_1^t E[XX^t] a_1 = a_1^t R a_1,$$

and therefore, the problem becomes as follows,

$$\begin{aligned} & \max_{a_1} a_1^t R a_1 \\ \text{s.a. } & a_1^t a_1 = 1 \end{aligned}$$

Finally, applying the *Lagrange Multiplier Theorem* for the calculation of constrained extremes, the problem is reduced to,

$$\max_{a_1} \{a_1^t R a_1 - \lambda(a_1^t a_1 - 1)\}$$



## Problem resolution - Step 1 (continuation)

Taking the derivative of the above expression with respect to  $a_1$  (matrix-wise and considering that  $R$  is symmetric) and setting it to zero,  $\frac{\partial(a_1^t R a_1 - \lambda(a_1^t a_1 - 1))}{\partial a_1} = 0$ , is obtained,

$$2R a_1 - 2\lambda a_1 = 0 \quad (1)$$

### Remark:

- The derivative of a quadratic form is:  $\frac{\partial(x^t A x)}{\partial x} = (A + A^t)x$  such that  $x \in \mathbb{R}^n, A \in M_n(\mathbb{R})$ .

It is easy to realize that  $a_1$  is the eigenvector associated with  $\lambda$ , the eigenvalue of  $R$ , since the previous expression is written as,

$$(R - \lambda I)a_1 = 0,$$

which determines the eigensubspace associated with  $\lambda$ . Finally, it is easy to deduce that  $\lambda$  is the variance of  $U_1$  since,

$$\text{Var}[U_1] = a_1^t R a_1 = \lambda a_1^t a_1 = \lambda,$$

multiplying (1) on the left by  $a_1^t$  and because  $a_1$  is unitary.

In conclusion, the first principal component is  $U_1 = a_1^t X$  with  $a_1$  the eigenvector associated with the eigenvalue of  $R$  with the highest magnitude.

## Problem resolution - Step 2

In this second step, the second principal component,  $U_2$ , is obtained, uncorrelated with the first principal component calculated previously, maximizing its variance.

To guarantee the existence of this maximum, bounding conditions must also be imposed on the weight vector, in this case  $a_2$  is also a unit vector.

$$\begin{aligned} & \max \text{Var}[U_2] \\ \text{s.a. } & \|a_2\| = a_2^t a_2 = 1 \\ & \text{cov}(U_1, U_2) = 0 \end{aligned}$$

Taking into account that  $X$  is a centred random vector,  $E[X] = 0$ , then  $E[a_2^t X] = 0$ , which implies that, as before,  $\text{Var}[U_2] = a_2^t R a_2$ .

Likewise  $\text{cov}(U_1, U_2) = E[a_1^t X a_2^t X] = E[a_1^t X X^t a_2] = a_1^t E[XX^t] a_2 = a_1^t R a_2$  and therefore the problem is as follows,

$$\begin{aligned} & \max_{a_2} a_2^t R a_2 \\ \text{s.a. } & a_2^t a_2 = 1 \\ & a_1^t R a_2 = 0 \end{aligned}$$

Finally, applying the *Lagrange Multiplier Theorem* for the calculation of constrained extremes, the problem is reduced to,

$$\max_{a_2} \{ a_2^t R a_2 - \lambda (a_2^t a_2 - 1) - \mu a_1^t R a_2 \}$$

## Problem resolution - Step 2 (continuation)

Taking the derivative of the above expression with respect to  $a_2$  (matrix-wise and considering that  $R$  is symmetric) and setting it to zero, is obtained,

$$2Ra_2 - 2\lambda a_2 - \mu Ra_1 = 0$$

**Remark:**

- The derivative of a linear form is:  $\frac{\partial(a^t x)}{\partial x} = a$  such that  $a, x \in \mathbb{R}^n$ .

Multiplying this expression on the left by  $a_1^t$ , it is derived,

$$2a_1^t Ra_2 - 2\lambda a_1^t a_2 - \mu a_1^t Ra_1 = 0$$

Considering that  $a_1^t Ra_2 = 0$  (it's the second constraint of the problem),  $a_1^t a_2 = 0$  (they are perpendicular), and  $a_1^t Ra_1 \neq 0$ , the expression becomes  $\mu a_1^t Ra_1 = 0$ , from which we deduce that  $\mu = 0$ . So the equation to solve is

$$2Ra_2 - 2\lambda a_2 = 0 \rightarrow (R - \lambda I)a_2 = 0, \quad (2)$$

from which it is again deduced that  $a_2$  is the eigenvector associated with the eigenvalue  $\lambda$  of the matrix  $R$ .

In the same way,  $Var[U_2] = a_2^t Ra_2 = \lambda a_2^t a_2 = \lambda$ , multiplying the previous equation on the left by  $a_2^t$  and considering that  $a_2$  is unitary.

In conclusion, the second principal component is  $U_2 = a_2^t X$ , where  $a_2$  is the eigenvector associated with the second eigenvalue of largest magnitude of matrix  $R$ .

## Problem resolution - Step 3 and onwards

In this third step, the third principal component,  $U_3$ , uncorrelated with the previously calculated first and second principal components, is obtained by maximizing its variance.

To ensure the existence of this maximum, bounding conditions on the weight vector must also be imposed, in this case, that  $a_3$  is also a unit vector.

$$\begin{aligned} & \max \text{Var}[U_3] \\ \text{s.a. } & \|a_3\| = a_3^t a_3 = 1 \\ & \text{cov}(U_1, U_3) = 0 \\ & \text{cov}(U_2, U_3) = 0 \end{aligned}$$

**Voluntary task:** to justify that  $a_3$  is the eigenvector associated with the third eigenvalue of largest magnitude of matrix  $R$ .

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## Práctica 1.1 de ACP

In this practice, a **first example of dimensionality reduction** is performed on a dataset. To complete it, you need to **download and run** the file [Practice\\_1.1\\_PCA.R](#) available on the PRADO platform.

### Topics covered:

- Conducting a preliminary exploratory analysis of the data to identify possible **missing data (NA - not available)** and **outliers**.
- **Making decisions and handling** missing data and outliers.
- Performing a **PCA (Principal Component Analysis)**
- Initial methods for **choosing the optimal number** of principal components.
- Interpretation of various **interesting graphical outputs** for this method.
- **R language:** loading data from an R package, *data.frame* object, graphical treatment of data, and construction of procedures or functions.

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## PCA Practice 1.2

In this practice, a **second example of dimensionality reduction** is performed on a dataset. To complete it, you need to **download and run** the file [Practice\\_1.2\\_PCA.R](#) available on the PRADO platform.

**The emphasis will be on:**

- Conducting a preliminary exploratory analysis of the data to identify possible **missing data** and **outliers**.
- **Making decisions and handling** missing data and outliers.
- Performing a **PCA (Principal Component Analysis)**.
- **Choosing the optimal number** of principal components.
- Interpretation of various **interesting graphical outputs** for this method.
- **R language:** RMarkdown notebook, loading external data files, methods **apply**, **tapply**, **width**, **by**, etc. for function debugging.
- Moving towards the **final report**.



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