Multivariate statistics

9 aprile 2025

Indice

Capitolo 1

Introduction

Remark 1 (Prerequisites). Random variables/vectors, linear models (least square principle, assumptions, R^2), matrix algebra (matrices, determinant, inverse, quadratic forms, eigenvalues-eigenvectors, Lagrange multipliers)

Remark 2 (Multivariate analysis situation). Large number of variables (p) observed on the same set of statistical units (n). Aim is to summarize somehow the data.

Important remark 1. Methods tackled in the course:

- *dimension reduction methods*: they share the aim to summarize the information contained in our data building new variables, limited in number, which can convey as much info as the original set. Among these the two methods we see are:
  - *Principal component*: is data transformation method. We transform data to obtain meaningful summary. Always feasible.
  - *Factor analysis*: is a *model* where we have to make assumptions: we fit and then check if model adequately is met.
- *discriminant analysis*: a supervised classification method. We have two (or more than two) groups and know that groups are different by characteristics (eg. healthy/diseased) collected in both groups. We want to find
  - a way to characterize the two groups: how different are which respect to which characteristic
  - a criteria to separate the two groups; to find a rule to assign a new observation (whose group membership is unknown) to one or the other group.
- *cluster analysis*: our aim is to find/create groups in the data (we have no previous groups as in discriminant analysis). Splitting should be done in order to have homogeneous units within group and different between groups

Important remark 2. Notation: for quantities referring to the population we use greek letters, while roman letters will be used for sample quantities. At the population level:

- the equivalent of S (variance/covariance matrix) is denoted as $\mathbf{\Sigma}$, which is called **population covariance matrix**
- the equivalent of the mean vector $\overline{x}$ will be μ
- the population analog of $\mathbf{R}$ (correlation matrix) is denoted by $\boldsymbol{\rho}$, the population correlation matrix

1.1 Matrices

1.1.1 Data matrix

The data matrix includes all data on observation were interested in:

- denoted as $\mathbf{X}$, it is $n \times p$ with n units (the generic one is unit j) and p variables (the generic one being i), be they categorical or numeric;
- each row correspond to a different unit;
- each column correspond to a variable: $X_1, \dots, X_p$;

$$\underset{n\times p}{\mathbf{X}} = \begin{bmatrix} x_{11} & \dots & x_{1i} & \dots x_{1p} \\ \dots & \dots & \dots & \dots \\ x_{j1} & \dots & x_{ji} & \dots x_{jp} \\ \dots & \dots & \dots & \dots \\ x_{n1} & \dots & x_{ni} & \dots x_{np} \end{bmatrix}$$

Remark 3. Multivariate analysis is concerned either with:

- studying the *relationships between variables* (PCA, Factor analysis and LDA focus on relationships between *columns*)
- studying the *similarities between units* (cluster analysis focus on the *row* of the data matrix).

Remark 4. Starting from the data matrix $\mathbf{X}$ a series of different matrices can be derived. We will first concentrate on the matrices dealing with relationships between variables, leaving the theme of measuring dissimilarities between units to when we will deal with clustering.

1.1.2 Mean vector

Important remark 3. For the moment we assume we're dealing with *numeric variables.*

We can associate to the data matrix the vector of means, $\overline{\mathbf{x}}$, a $p \times 1$ column vector containing column means:

$$\underset{p\times 1}{\overline{\mathbf{x}}} = \begin{bmatrix} \overline{x}_1 \\ \vdots \\ \overline{x}_i \\ \vdots \\ \overline{x}_p \end{bmatrix} = \left(\frac{\mathbf{1}_n^\top \mathbf{X}}{n}\right)^\top = \left(\frac{1}{n}\mathbf{1}_n^\top \mathbf{X}\right)^\top = \frac{1}{n}\mathbf{X}^\top \mathbf{1}_n$$

To obtain it in matrix form by pre-multiplying $\mathbf{X}$ by a row vector of all 1 we obtain the sum of all elements in column, then we divide by n to have the mean and finally we transpose to have a column vector.

1.1.3 Mean centered matrix

In certain applications it might be useful to express the variables as deviations from the mean. The mean vector can be used to obtain the mean centered data matrix, $\tilde{\mathbf{X}}$:

$$\underset{n\times p}{\tilde{\mathbf{X}}} = \begin{bmatrix} \tilde{x}_{11} & \dots & \tilde{x}_{1i} & \dots & \tilde{x}_{1p} \\ \dots & \dots & \dots & \dots & \\ \tilde{x}_{j1} & \dots & \tilde{x}_{ji} & \dots & \tilde{x}_{jp} \\ \dots & \dots & \dots & \dots & \\ \tilde{x}_{n1} & \dots & \tilde{x}_{ni} & \dots & \tilde{x}_{np} \end{bmatrix} = \begin{bmatrix} x_{11}-\overline{x}_1 & \dots & x_{1i}-\overline{x}_i & \dots & x_{1p}-\overline{x}_p \\ \dots & \dots & \dots & \dots & \dots \\ x_{j1}-\overline{x}_1 & \dots & x_{ji}-\overline{x}_i & \dots & x_{jp}-\overline{x}_p \\ \dots & \dots & \dots & \dots & \dots \\ x_{n1}-\overline{x}_1 & \dots & x_{ni}-\overline{x}_i & \dots & x_{np}-\overline{x}_p \end{bmatrix}$$

How to obtain $\tilde{\mathbf{X}}$ from $\mathbf{X}$ and $\overline{\mathbf{x}}$? The difference between two matrix can be obtained only if we have matrix of the same size; we need to subtract from $\mathbf{X}$ a matrix $\overline{\mathbf{X}}$ where each row is a copy of $\overline{\mathbf{x}}$:

$$\underset{n\times p}{\overline{\mathbf{X}}} = \underset{n\times 1}{\mathbf{1_n}}\underset{1\times p}{\overline{\mathbf{x}}^\top} = \begin{bmatrix} \overline{x}_1 & \dots & \overline{x}_i & \dots & \overline{x}_p \\ \dots & \dots & \dots & \dots & \dots \\ \overline{x}_1 & \dots & \overline{x}_i & \dots & \overline{x}_p \\ \dots & \dots & \dots & \dots & \dots \\ \overline{x}_1 & \dots & \overline{x}_i & \dots & \overline{x}_p \end{bmatrix}$$

Therefore

$$\tilde{\mathbf{X}} = \mathbf{X} - \mathbf{1_n}\overline{\mathbf{x}}^\top = \mathbf{X} - \frac{1}{n}\mathbf{1}_n\mathbf{1}_n^\top\mathbf{X} = \underbrace{\left(\mathbf{I}_n - \frac{1}{n}\mathbf{1}_n\mathbf{1}_n^\top\right)}_{\mathbf{A}}\mathbf{X}$$

where in the final passage we collected $\mathbf{X}$ (to the right) and added the identity matrix which leaves the product unchanged.

Remark 5. We have that:

- Mean vector of $\tilde{\mathbf{X}}$ is $\mathbf{0}$
- $\tilde{\mathbf{X}}$ defines a translation of the origin of the original reference system. The shape of the point cloud remains unchanged, but the origin of the axes is moved to $\overline{\mathbf{x}}$.

Definition 1.1.1 (Centering matrix). $\mathbf{A}$ is usually called the *centering matrix*: if we pre-multiply a matrix for $\mathbf{A}$ we obtained the mean centered matrix;

Important remark 4. $\mathbf{A}$ is very interesting from the algebraic point of view:

- is $n \times n$;
- is *symmetric*: coincides with its transpose since difference of two symmetric matrix ($\mathbf{1}_n\mathbf{1}_n^\top$ transposed is the same and $\mathbf{I}_n$ is symmetric)
- is *idempotent*: $\mathbf{A} = \mathbf{A}^2$

1.1.4 Standardized data matrix

If one wants to eliminate the effect of different scales on the observed variables, one can resort on this matrix.
To standardize a single cell we have

$$z_{ji} = \frac{x_{ji} - \overline{x}_i}{s_i}$$

where the numerator is clearly taken from $\tilde{X}$ while at the denominator we have the standard deviation of i-th column/variable. To compute in matrix form how to divide each column by its standard deviation?
First we build a diagonal matrix which have the variances s_i^2 on the main diagonal

$$\underset{p\times p}{\mathbf{D}} = \begin{bmatrix} s_1^2 & \dots & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & s_i^2 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & \dots & s_p^2 \end{bmatrix}$$

then we define its power of $-1/2$

$$\underset{p\times p}{\mathbf{D}^{-\frac{1}{2}}} = \begin{bmatrix} \frac{1}{s_1} & \dots & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \frac{1}{s_i} & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & \dots & \frac{1}{s_p} \end{bmatrix}$$

Thus we obtain the standardized data matrix post-multiplying the standardized data matrix by $\mathbf{D}^{-\frac{1}{2}}$ (equivalent to dividing each column by its standard deviation)

$$\underset{n\times p}{\mathbf{Z}} = \underbrace{\begin{bmatrix} x_{11} - \overline{x}_1 & \dots & x_{1i} - \overline{x}_i & \dots & x_{1p} - \overline{x}_p \\ \dots & \dots & \dots & \dots & \dots \\ x_{j1} - \overline{x}_1 & \dots & x_{ji} - \overline{x}_i & \dots & x_{jp} - \overline{x}_p \\ \dots & \dots & \dots & \dots & \dots \\ x_{n1} - \overline{x}_1 & \dots & x_{ni} - \overline{x}_i & \dots & x_{np} - \overline{x}_p \end{bmatrix}}_{\tilde{\mathbf{X}}} \underbrace{\begin{bmatrix} \frac{1}{s_1} & \dots & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \frac{1}{s_i} & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & \dots & \frac{1}{s_p} \end{bmatrix}}_{\mathbf{D}^{-\frac{1}{2}}}$$

Thus, at the same time

$$\underset{n\times p}{\mathbf{Z}} = \tilde{\mathbf{X}}\mathbf{D}^{-\frac{1}{2}} = \mathbf{A}\mathbf{X}\mathbf{D}^{-\frac{1}{2}}$$

Remark 6. Each column of $\mathbf{Z}$ has zero mean and unit variance.

Remark 7. We can work with raw, mean centered or standardized variables: which matrix is better to use is something we'll discuss.

1.1.5 (Variance-)Covariance matrix

Remark 8. The covariance between two variables X_k and X_h is defined as

$$\text{Cov}\,(X_k, X_h) = \frac{\sum_{j=1}^{n}(x_{jk} - \overline{x}_k)(x_{jh} - \overline{x}_h)}{n} = \frac{1}{n}\sum_{j=1}^{n}(\tilde{x}_{jk})(\tilde{x}_{jh}) = \frac{1}{n}\tilde{\mathbf{x}}_k^\top \tilde{\mathbf{x}}_h$$

where $\tilde{\mathbf{x}}_k$ and $\tilde{\mathbf{x}}_h$ are the k-th and h-th columns of $\tilde{\mathbf{X}}$ respectively.

Important remark 5. It is worth remembering that

- $\text{Cov}\,(X_k, X_h) = \text{Cov}\,(X_h, X_k)$
- the covariance between a variable and itself is but the variance of the variable itself
- numerator of variance and covariance (excluding $\frac{1}{n}$) are called *deviance* and *codeviance*

Variances and covariances can then be summarized in the so called covariance matrix $\mathbf{S}$, a $p \times p$ matrix that has variances on the main diagonal and covariances outside

$$\underset{p\times p}{\mathbf{S}} = \begin{bmatrix} \text{Var}\,[X_1] & \dots & \text{Cov}\,(X_1, X_j) & \dots & \text{Cov}\,(X_1, X_p) \\ & & \text{Var}\,[X_i] & \dots & \text{Cov}\,(X_i, X_p) \\ & & & & \text{Var}\,[X_p] \end{bmatrix} = \begin{bmatrix} s_1^2 & \dots & s_{1i} & \dots & s_{1p} \\ & & s_i^2 & \dots & s_{ip} \\ & & & & s_p^2 \end{bmatrix}$$

If we have p variables:

- the number of variances is obviously p (on the diagonal)
- the number of (unique) covariances, which fill the upper matrix, is the sum of the first p natural number which is

  $$ncovs = \frac{p(p-1)}{2}$$

  eg with 3 variables we have 3 unique covariances

Important remark 6 (Matrix form derivation). Let's see the component for a generic element on the diagonal (variance) and out of it (covariance) respectively

$$\text{Var}\,[X_i] = s_i^2 = \frac{\sum_{j=1}^{n}(x_{ji} - \overline{x}_i)^2}{n}, \quad \text{Cov}\,(X_i, X_l) \quad = s_{il} = \frac{\sum_{j=1}^{n}(x_{jl} - \overline{x}_l)(x_{ji} - \overline{x}_i)}{n}$$

To obtain $\mathbf{S}$ the main ingredient are the element of matrix $\tilde{\mathbf{X}}$ of deviations from the mean, which are multiplied by themselves and then divided by n so

$$\mathbf{S} = \frac{1}{n}\tilde{\mathbf{X}}^\top\tilde{\mathbf{X}}$$

Remark 9. Generally $\tilde{\mathbf{X}}^\top\tilde{\mathbf{X}}$ is called **deviance/codeviance matrix** (numerators of variances/covariances)

Remark 10. Here we used the biased version of the matrix (with n at denominator of each element, not $(n-1)$. We could define as well

$$\widehat{\mathbf{S}} = \frac{1}{n-1}\tilde{\mathbf{X}}^\top\tilde{\mathbf{X}}$$

which is the *unbiased covariance matrix.*

For our purposes using one or the other is the same but if needed to change between the two is done easily by multiplying by n and divide by $n-1$ or viceversa

Important remark 7 (Properties). It's

- *squared* $p \times p$
- *symmetric* (so people usually write just the upper triangular part): we know this from property of covariance but as well if we transpose above we obtain the same
- is *positive semi definite*
- it's trace is the called t*otal variance*:

$$\operatorname{Tr} \mathbf{S} = \sum_{i=1}^{p} \operatorname{Var}[X_i]$$

Dimostrazione. To prove a matrix is positive semi definite we can procede in two ways

- prove its eigenvalues are $>= 0$
- prove the determinant of the matrix and determinant of all the minors are $>= 0$

To prove **S** is positive semi-definite go this second way. In the simple case of just two variables, let's consider just two mean-centered variables

$$\mathbf{S} = \frac{1}{n}\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}} = \frac{1}{n}\begin{bmatrix} Dev(X_1) & Codev(X_1, X_2) \\ Codev(X_1, X_2) & Dev(X_2) \end{bmatrix}$$

where $Dev(X_1)$ is the deviance (numerator of the variance) while $Codev(X_1, X_2)$ is the codeviance (numerator of covariance).
For what concerns:

- determinant of **S**:

$$\det \mathbf{S} = Dev(X_1) \cdot Dev(X_2) - Codev^2(X_1, X_2)$$

  To check the inequality

$$\begin{aligned} Dev(X_1) \cdot Dev(X_2) - Codev^2(X_1, X_2) &\geq 0 \\ Dev(X_1) \cdot Dev(X_2) &\geq Codev^2(X_1, X_2) \end{aligned}$$

  By dividing both sides by $Dev(X_1) \cdot Dev(X_2)$ (and reverting order) we have that determinant is ≥ 0 as long as

$$\begin{aligned} &\frac{Codev(X_1, X_2)}{Dev(X_1)Dev(X_2)} \leq 1 \\ &r_{12}^2 \leq 1 \end{aligned}$$

  where r_{12}^2 is the R^2, the square of correlation coefficient between the two variables r_{12},
  By definition the R^2 is always ≤ 1, being the correlation coefficient in the range -1 to 1 So this is true by definition and thus $\det \mathbf{S} \geq 0$

- the determinant of its minor is non negative: here we have just 1 minor obtained by canceling the first row and first column. The minor is scalar/matrix with just $dev(x_2)$ and its determinant is just scalar itself

$$\det([dev(x_2)]) = dev(x_2) \geq 0$$

$\square$

Important remark 8. The fact that S is positive-semidefinite, that is cannot have negative eigenvalues. have a statistical interpretation since we will se that eigenvalue are variances (that cannot be negative).
Negative eigenvalue for $\mathbf{S}$ means something gone wrong in the computation

1.1.6 Correlation matrix

The covariance between two standardized variables Z_i, Z_l is the correlation between the corresponding unstandardized ones X_i, X_l since:

$$\begin{aligned}
\operatorname{Cov}(Z_i, Z_l) &= \frac{\sum_{j=1}^n (z_{ji} - \overline{z}_i)(z_{jl} - \overline{z}_l)}{n} \overset{(1)}{=} \frac{\sum_{j=1}^n z_{ji} - z_{jl}}{n} (= \frac{1}{n}\mathbf{z}_i^\top \mathbf{z}_l) \\
&= \frac{\sum_{j=1}^n (x_{ji} - \overline{x}_i)(x_{jl} - \overline{x}_l)/\sqrt{\operatorname{Var}[X_i]\operatorname{Var}[X_l]}}{n} \\
&= \frac{\sum_{j=1}^n (x_{ji} - \overline{x}_i)(x_{jl} - \overline{x}_l)/n}{\sqrt{\operatorname{Var}[X_i]\operatorname{Var}[X_l]}} = \frac{\operatorname{Cov}(X_i, X_l)}{\sqrt{\operatorname{Var}[X_i]\operatorname{Var}[X_l]}} \\
&= \operatorname{Corr}(X_i, X_l) = r_{il}
\end{aligned}$$

where in (1) considering that standardized variables has zero mean.

Definition 1.1.2. Putting all the correlations between the p variables in the correlation matrix $\mathbf{R}$ we end with:

$$\underset{p\times p}{\mathbf{R}} = \begin{bmatrix} 1 & \dots & r_{1i} & \dots & r_{1p} \\ & & 1 & \dots & r_{ip} \\ & & & & 1 \end{bmatrix}$$

where outside the main diagonal there are linear correlation coefficients between variables (-1 to 1), while on the main diagonal all are 1 (correlation between variable with itself).

Important remark 9 (Computation). To compute it, being the correlation of the unstandardized variable the covariance of the standardized ones, we can procede as done for variance covariance matrix (but starting from the standardized variable matrix instead of the mean centered):

$$\begin{aligned}
\mathbf{R} = \operatorname{Cov}(\mathbf{Z}) = \frac{1}{n}\mathbf{Z}^\top\mathbf{Z} = \frac{1}{n}\mathbf{D}^{-1/2}\tilde{\mathbf{X}}^\top\tilde{\mathbf{X}}\mathbf{D}^{-1/2} = \mathbf{D}^{-1/2}\underbrace{\frac{1}{n}\tilde{\mathbf{X}}^\top\tilde{\mathbf{X}}}_{\mathbf{S}}\mathbf{D}^{-1/2} \\
= \mathbf{D}^{-1/2}\mathbf{S}\mathbf{D}^{-1/2}
\end{aligned}$$

it turns out that can be obtained the variance covariance matrix (numerator of corr) by both std of one and the other variables, in matrix form, just bye pre and postmultiply by $\mathbf{D}^{-1/2}$.
So we can obtain $\mathbf{R}$ both from $\mathbf{S}$ or from $\mathbf{Z}$

Important remark 10 (Properties). Since $\mathbf{R}$ is a covariance matrix it has the property of any covariance matrix so

- squared $p \times p$
- symmetric (if we transpose we get the same)
- positive semi definite

Remark 11 (Some final remarks). Either covariance matrix between standardized variables is the correlation matrix or the correlation matrix can be thaught as the covariance matrix of standardized variables.
Every time we work with $\mathbf{R}$ it's like we're working with (relationship between) standardized variables.
In study we can work either

- with $\mathbf{S}$
- with $\mathbf{R}$ if we want get rid of different measurement units

1.2 Multivariate random variables and derived linear combinations

The data matrix $\mathbf{X}$ may be thought of as describing a sequence of n empirical realizations of a p-dimensional random vector $\mathbf{x}^\top$.
In the following we will first describe multivariate statistical methods considering random vectors (i.e. at the population level) and then we will derive their sample counterpart.
Let's assume we are dealing with a p-dimensional random vector $\mathbf{x}$; we will denote

- by μ its p-dimensional expectation
- by $\mathbf{\Sigma}$ its $p \times p$ covariance matrix. It is worth remembering that, for mean centered random variables, $\mathbf{\Sigma} = \mathbb{E}\left[\mathbf{x}\mathbf{x}^T\right]$.

Single linear combinations Most of the multivariate statistical methods we will deal with in the following are based on *linear combinations of the components of a random vector*. We will define as a single linear combination as

$$y = \mathbf{a}^\top \mathbf{x}$$

where $\mathbf{a}$ is the p-dimensional vector of coefficients. Note that y is a scalar random variable.
The expected value and the variance of a single linear combination will be:

$$\begin{aligned}\mathbb{E}[y] &= \mathbb{E}\left[\mathbf{a}^\top \mathbf{x}\right] = \mathbf{a}^\top \mathbb{E}[\mathbf{x}] = \mathbf{a}^\top \mu \\ \operatorname{Var}[y] &= \operatorname{Var}\left[\mathbf{a}^\top \mathbf{x}\right] = \mathbf{a}^\top \operatorname{Var}[\mathbf{x}]\,\mathbf{a} = \mathbf{a}^\top \mathbf{\Sigma}\mathbf{a}\end{aligned}$$

Note that, because of the properties of the covariance matrix, the variance of a single linear combination is a *positive semi definite quadratic form.*
It is interesting to study its properties as the vector a varies: let's consider again the simple case consisting of two variables only and a generic covariance $\Sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{bmatrix}$.
After suitably performing the scalar product we obtain:

$$\mathrm{Var}\left[y\right] = \mathbf{a}^\top \mathbf{\Sigma} \mathbf{a} = \begin{bmatrix} a1 & a2 \end{bmatrix} \begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{bmatrix} \begin{bmatrix} a1 \\ a2 \end{bmatrix} = a_1^2 \sigma_{11} + 2a_1 a_2 \sigma_{12} + a_{22}\sigma_{22}$$

If we read this variance:

- as a function of a_1 we easily recognize, in the polynomial of degree 2, the equation of a parabola. The coefficient of a_1^2 is positive since it is a variance, the equation describes therefore a concave up parabola;
- the same happens if we read the variance as a function of a_2.

This means that, as a varies, $\mathrm{Var}\left[y\right]$ does never reach a finite maximum, but only a minimum.

Multiple linear combination if interested in more than one linear combination, say m, the vectors of coefficients will be the columns of a $p \times m$ matrix $\mathbf{A}$; the m linear combinations will be the components of the m-dimensional random vector obtained by

$$\mathbf{y} = \mathbf{A}^\top \mathbf{x}$$

The expected value and the variance of multiple linear combinations will be:

$$\mathbb{E}\left[\mathbf{y}\right] = \mathbb{E}\left[\mathbf{A}^\top \mathbf{x}\right] = \mathbf{A}^\top \,\mathbb{E}\left[\mathbf{x}\right] = \mathbf{A}^\top \mu$$
$$\mathrm{Var}\left[\mathbf{y}\right] = \mathrm{Var}\left[\mathbf{A}^\top \mathbf{x}\right] = \mathbf{A}^\top \,\mathrm{Var}\left[\mathbf{x}\right] \mathbf{A} = \mathbf{A}^\top \mathbf{\Sigma} \mathbf{A}$$

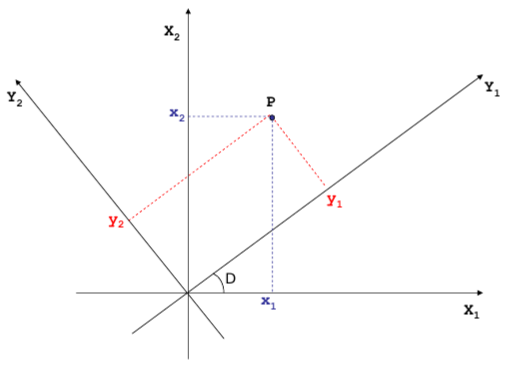
Orthogonal combinations Linear combinations defined by an *orthogonal* matrix $\mathbf{A}$ describe an axes *rotation in the multidimensional space.* A simpler two variable case may help in understanding why.
Figure 1.1 presents the coordinates of point P, both in the original reference system X_1, X_2 and in the new reference system Y_1, Y_2 obtained after rotating the system X_1, X_2 by an angle α.
The coordinates of P in the original reference system are (x_1, x_2), while in in the rotated reference system (y_1, y_2) and can be obtained from the original ones as

$$y_1 = x_1 \cos\alpha + x_2 \sin\alpha$$
$$y_2 = -x_1 \sin\alpha + x_2 \cos\alpha$$

or, with a notation coherent with the one we used before as:

$$y_1 = \mathbf{a}_1^\top \mathbf{x}$$
$$y_2 = \mathbf{a}_2^\top \mathbf{x}$$

where, because of $\sin^2\alpha + \cos^2\alpha = 1$ both $\mathbf{a}_1$ and $\mathbf{a}_2$ are unit norm vectors.
The rotated coordinates are therefore a linear combination of the original ones.



(a)

Figura 1.1: Axes rotation

Example 1.2.1. Given a bi-dimensional random vector $\mathbf{x}^\top = (x_1, x_2)$ with expected value $\mu^\top = (\mu_1, \mu_2)$ and covariance matrix

$$\Sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{bmatrix}$$

consider the two linear combinations

$$y_1 = x_1 - x_2$$
$$y_2 = x_1 + x_2$$

and derive the expected value and the covariance (the solution will be provided in class).

Example 1.2.2. Consider three independent standardized variables Z1 , Z2 , Z3 . Assume you transform them as follows obtaining three new variables Y1 , Y2 , Y3 :

$$Y_1 = Z_1$$
$$Y_2 = Y_1 + 0.01Z_2$$
$$Y_3 = 10Z_3$$

Derive the covariance matrix of the new Y variables.

1.3 Lab

To doing matrix manipulation let's consider the dataset `job_perf` Data contain observations on fifty police officers that were rated by their supervisors in 6 categories as part of standard police departmental administrative procedure:

- `commun`: Communication Skills

- `probl_solv`: Problem Solving
- `logical`: Logical Ability
- `learn`: Learning Ability
- `physical`: Physical Ability
- `appearance`: Appearance

To do matrix computation we convert it to matrix and extract number of units which is neede in the following

```
# matrix computation
job <- read.table("data/job_perf.txt", header = TRUE)
head(job)

##   commun probl_solv logical learn physical appearance
## 1     12         52      20    44       48         16
## 2     12         57      25    45       50         16
## 3     12         54      21    45       50         16
## 4     13         52      21    46       51         17
## 5     14         54      24    46       51         17
## 6     14         48      20    47       51         18

X <- as.matrix(job)
n <- nrow(X)
```

1.3.1 Mean centered matrix

```
C <- diag(n) - (1/n) * rep(1, n) %*% t(rep(1, n)) # mean centering matrix
Xc <- C %*% X # centered data
colMeans(Xc) ## check it's centered (mean should be 0)

##        commun    probl_solv       logical         learn      physical
## -5.639933e-16  6.679102e-15 -3.792522e-15 -9.414691e-16  1.059597e-14
##    appearance
## -2.646772e-15
```

1.3.2 Covariance matrix

```
## covariance matrix
(S <- 1/n * t(Xc) %*% Xc) ## S is 6x6

##            commun probl_solv logical  learn physical appearance
## commun     7.3776     0.8512  1.5064 7.4896   6.3312     7.7992
## probl_solv 0.8512     5.6944  2.1368 0.9552   0.9344     0.9104
## logical    1.5064     2.1368  6.0596 1.5944   1.5168     1.5788
## learn      7.4896     0.9552  1.5944 7.8816   6.5752     8.0832
## physical   6.3312     0.9344  1.5168 6.5752   5.6944     6.8504
## appearance 7.7992     0.9104  1.5788 8.0832   6.8504     8.7764

## using cov we get the unbiased covariance so to obtain the same..
cov(X) * (n-1) / n

##            commun probl_solv logical  learn physical appearance
## commun     7.3776     0.8512  1.5064 7.4896   6.3312     7.7992
## probl_solv 0.8512     5.6944  2.1368 0.9552   0.9344     0.9104
## logical    1.5064     2.1368  6.0596 1.5944   1.5168     1.5788
## learn      7.4896     0.9552  1.5944 7.8816   6.5752     8.0832
## physical   6.3312     0.9344  1.5168 6.5752   5.6944     6.8504
## appearance 7.7992     0.9104  1.5788 8.0832   6.8504     8.7764
```

1.3.3 Standardized data

```
## for the standardized data: D is diagonal matrix that has variances
D <- diag(diag(S))
# diag(S) only extracts the diagonal of our matrix (which has the variances):
# we use another diag to make a diagonal matrix

## do do the ^{-1/2}  we have to do solve which correspond to -1
Z <- Xc %*% solve(D^0.5)

## check that standardized (mean = 1, sd = var = 1)
round(colMeans(Z), 5) # all 0

## [1] 0 0 0 0 0 0

apply(Z, 2, var) # more or less all standardized

## [1] 1.020408 1.020408 1.020408 1.020408 1.020408 1.020408
```

1.3.4 Correlation matrix

```
## can be found in different ways (covaraince of standardized data or starting
## from the covaraince matrix)

(R <- 1/n * t(Z) %*% Z) #cov: on diagonal 1 (it's a corr)

##           [,1]      [,2]      [,3]      [,4]      [,5]      [,6]
## [1,] 1.0000000 0.1313258 0.2252998 0.9821863 0.9767974 0.9692466
## [2,] 0.1313258 1.0000000 0.3637625 0.1425815 0.1640910 0.1287805
## [3,] 0.2252998 0.3637625 1.0000000 0.2307109 0.2582155 0.2164945
## [4,] 0.9821863 0.1425815 0.2307109 1.0000000 0.9814717 0.9718918
## [5,] 0.9767974 0.1640910 0.2582155 0.9814717 1.0000000 0.9690222
## [6,] 0.9692466 0.1287805 0.2164945 0.9718918 0.9690222 1.0000000
```

```
(R <- solve(D^0.5) %*% S %*% solve(D^0.5)) ## same results obtained with D^{-1/2} S D^{-1/2}

##           [,1]      [,2]      [,3]      [,4]      [,5]      [,6]
## [1,] 1.0000000 0.1313258 0.2252998 0.9821863 0.9767974 0.9692466
## [2,] 0.1313258 1.0000000 0.3637625 0.1425815 0.1640910 0.1287805
## [3,] 0.2252998 0.3637625 1.0000000 0.2307109 0.2582155 0.2164945
## [4,] 0.9821863 0.1425815 0.2307109 1.0000000 0.9814717 0.9718918
## [5,] 0.9767974 0.1640910 0.2582155 0.9814717 1.0000000 0.9690222
## [6,] 0.9692466 0.1287805 0.2164945 0.9718918 0.9690222 1.0000000

cor(X) ## same again

##               commun probl_solv   logical     learn  physical appearance
## commun     1.0000000  0.1313258 0.2252998 0.9821863 0.9767974  0.9692466
## probl_solv 0.1313258  1.0000000 0.3637625 0.1425815 0.1640910  0.1287805
## logical    0.2252998  0.3637625 1.0000000 0.2307109 0.2582155  0.2164945
## learn      0.9821863  0.1425815 0.2307109 1.0000000 0.9814717  0.9718918
## physical   0.9767974  0.1640910 0.2582155 0.9814717 1.0000000  0.9690222
## appearance 0.9692466  0.1287805 0.2164945 0.9718918 0.9690222  1.0000000
```

Capitolo 2

Cluster analysis

So far we focused on the columns (variances mean covariances). Now we start to see the dataset row-wise, our focus is to measure similarity or dissimilarity of units. I want to read the data matrix row-wise and compare each unit to each other units.

We need to define some metrics and matrices before proceeding. Disclaimer: we have more object that letters in our alphabet sometimes we use the same letter but the context will clarify Here the matrix D will be used as distance matrix (previously used as diagonal matrix)

2.1 Distance matrix

The distance or dissimilarity matrix $\mathbf{D}$ is $n \times n$ and comprises all the distances/dissimilarity between units belonging to the sample. In most cases it is symmetric (if we use distance, which are symmetric) but not need to be so.
Let's consider distance function between units. The various type depends on the kind of data they apply

2.1.1 Distances

2.1.1.1 All numeric variables

How to compare units where all the variable are numerical? With all numeric variables we can think of each unit as a point in the p-dimensional space

Example 2.1.1. In two dimensions

```
         height weight
vadim      182     80
daulet     185     87
```

data can be represented as point in the two dimensional space.
With tree variables we have points in space, with p-variable the unit are point in the p-dimensional variable.

Since data are mapped to points i can measure the difference between units as distance between corresponding points the more different they are the more distant the corresponding will be. while if the points are overlapping the distance will be 0

There are many definition of distances for all quantitative variables

- **euclidean distance**: in the 2-dimensional space is the length of the segment joining the two points (just applying pitagora's theorem). n general the distance between unit j and h is

  $$d_{jh} = \sqrt{\sum_{i=1}^{p} (x_{ji} - x_{hi})^2}$$

  which is also called the L_2-norm

- city-block/Manhattan distance:

  $$d_{jh} = \sum_{i=1}^{p} |x_{ji} - x_{hi}|$$

  The name comes from the fact that in Manhattan we can't walk diagonal so we need to count the segments of streets which separates two point. Also called L_1-norm

- **Minkowski distance**: the previous are specialization of the following family of distances

  $$d_{jh} = \sqrt[m]{\sum_{i=1}^{p} |x_{ji} - x_{hi}|^m}$$

  If $m = 1$ we obtain the city block distance, while if $m = 2$ we obtain the Euclidean distance.
  In general larger and values for m put larger weights on large differences (difference is large and raise to a large power take power on the other differences on other variables).

Example 2.1.2. To see the impact of increasing m on variables relevance see

$$\text{manhattan:} \quad d_{vd} = |182 - 185| + |80 - 87| = 3 + 7 = 10$$
$$\text{euclidean:} \quad d_{vd} = \sqrt{(182 - 185)^2 + (80 - 87)^2} = \sqrt{9 + 49} = \sqrt{58} = 7.62$$

Going from Manhattan to Euclidean distance become smaller but the importance of weight variable (were the difference between units is higher) become bigger

2.1.1.2 All binary variables

Example 2.1.3. Suppose

```
        brother  smoke  likebeer likechocolate
vadim         1      0         1             0
daulet        1      0         0             1
```

V D	1	0	
1	a	b	
0	c	d	
			p

Tabella 2.1: The mf counts table

How to measure how units are similar with respect to p binary variables. A table such as 2.1 is constructed with the count of variable where the two units have agreement or disagreement where

- a: number of times (variables) where units agree on 1
- d: number of times the units agree on 0
- b: n of times unit i shows the 1 while the unit h show 0 (disagree)
- c: n of times unit i shows the 0 while the unit h show 1 (disagree)

All sum of all the entries will be p, the number of variable. In the example above we have $a = b = c = d = 1$. Basing ourselves on the matrix we have several dissimilarity coefficients:

1. *simple dissimilarity coefficient*

$$\begin{aligned} d_{ih} &= \frac{\text{n. disagree}}{n.\ variables} = \frac{b+c}{a+b+c+d} \\ &= 1 - s_{ih} = 1 - \frac{a+d}{a+b+c+d} \end{aligned}$$

   where s_{ih} is called simple similarity coefficient.
   It's called *dissimilarity* and not *distance* because a distance function requires to be positive symmetric AND to satisfy triangular inequality; this function does not satisfy the third property (dissimilarity usually don't)

2. *Jaccard coefficient*: is defined as

$$d_{ih} = \frac{a}{a+b+c}$$

   These measures were defined for taxonomy studies and the used to compare different animals. In these cases there are many agreement on not having certain characteristics. But having agreement on not having wings (cows and snake) does not necessarily mean that two animals (units) are similar.
   Generalizing Jaccard consider in many cases the agreement on null non necessarily means similarity. Jaccard invented the jaccard coefficient, which eliminates in the numerator and denominator the agreement on null

Example 2.1.4. In our example, with $a = b = c = d$ we have that the simple dissimilarity between vadim and daulet is

$$d_{vd} = \frac{2}{4} = 0.5$$

so the two units are identical with respect to half o characteristics considered.

2.1.1.3 All categorical variables

Example 2.1.5. Suppose

```
        phone   fav.team  zodiac blood
vadim  iphone barcellona  gemini    A-
daulet iphone juventus      lion    B+
```

Difference between the units is just the number of agreement/number of variable

$$d_{jh} = \frac{\text{n.agreement}}{\text{n.variables}} = \frac{\text{n.agreement}}{p}$$

However this is a poor measure of similarity which does not take account the number of levels of each variables (eg is easy to have distance in zodiac sign more easy in the phone iphone vs android)

2.1.1.4 Mixed types

Example 2.1.6.

```
         height  weight   phone brother beer
 vadim    182       80  iphone       1    1
daulet    185       87  iphone       1    0
```

A popular measure here is the Gower's dissimilarity coefficient which is defined as the complement of similarity measure

$$d_{jh} = 1 - s_{jh}$$
$$s_{jh} = \frac{\sum_{i=1}^{p} s_{jhi} \cdot \delta_{jhi}}{\sum_{i=1}^{p} \delta_{jhi}}$$

Regarding

- δ_{jhi} which is an indicator defined as

  $$\delta_{jhi} = \begin{cases} 1 & \text{if comparison between unit } j \text{ and } h \text{ is possible for variable } i \\ 0 & \text{otherwise} \end{cases}$$

  This indicator take into account the very likely situation that for 1 unit a piece of information is lacking: if we have missing values the two units cannot be compared and in this case it is impossible to use data to tell difference. If all the variables can be compared at the numerator we have p, which is a counter where both the units are non-missing.
  δ_{jhi} is a simply way to taking into account missingness

- the similarity s_{jhi} quantity is defined separatedly for *each variable*. If the variables are

  - numeric

    $$s_{jhi} = \frac{1 - |x_{ji} - x_{hi}|}{\text{range of } x_i} = 1 - \frac{x_{ji} - x_{hi}}{max(x_i) - min(x_i)}$$

– binary

$$s_{jhi} = \begin{cases} 1 & \text{the units show the same level} \\ 0 & \text{otherwise} \end{cases}$$

Example 2.1.7. Eg for height which is numerical

$$s_{vd,height} = 1 - \frac{|182 - 185|}{190 - 160} = 1 - \frac{3}{30} = \frac{9}{10}$$

where 190 and 160 were the height of taller and smaller in class. So being 9/10 the two units are very similar (close to 1).
In case of considering the similarity of the most distant units we have

$$s_{vd,height} = 1 - \frac{|190 - 160|}{190 - 160} = 0$$

and we have max difference.
For what concerns the similarity in weight

$$s_{vd,weight} = 1 - \frac{|87 - 80|}{90 - 48} = 1 - \frac{7}{46} = \frac{5}{6} = 0.83$$

where 90 and 48 are the weights of the fatter and thinner in class. So 0.83 is still highly similar units.
Thus finally overall we have that the Gower dissimilarity is

$$d_{dv} = 1 - s_{dv} = 1 - \frac{0.9 + 0.83 + 1 + 0}{4} = 1 - 0.68 = 0.32$$

Dissimilarity between the two units is 0.32 and we do the same things for all the units

2.2 Clustering

A *cluster* is a group of unit.

Goal of this analysis to find groups of units that are similar within group and separate/different between as much as we can (wrt the variable we take into account).

Important *starting point* in variable selection: we have to choose carefully the charateristics to analyze (same set of units can provide very different information).

Cluster analysis is composed by a very broad sets of techniques: one can define groups in many way and thus obtain many different solutions.

The most traditional way cluster analysis is performed we have two main method:

- *hierarchical methods*: the methods work by building a series of nested classification (small group inside larger and so on). we don't have a single clustering
- partitioning methods:

Hierarchical methods can be divided in two family (based on the way on which is builded):

- *agglomerative methods* (bottom-up) (which is the one we will study): start from n cluster group each composed by 1 unitm, and we put clusters together/merge them until we obtain the big group. The procedure/merging process is depicted by a dendrogram

- *divisive methods* (top-down): splitting in subgroups up to when each group has 1 unit.
  Most famous divisive methods is due to Edwards and Cavalli Sforza (biological domani, numerical variables only based onthe decomposition of total sum of square in the within/between, in order to have the smallest within and larger between). One goes on up to when variability is zero in each group ($n = 1$ for each).
  This approach is not very much used because very computational demanding (we have to try each splitting) and furthermore only for numerical variabile. Finally if we make mistakes in the first stages, the error goes on and on (contrary to agglomerative)

A group/cluster of just 1 unit is called *singleton*.

2.3 Hierarchical agglomerative methods

We know how to compute the dissimilarity between pair of units; now we need a measure *distance between groups* (to make them as distant possible): according on how to define the similarity of groups we have different clustering solutions. For group dissimilarity we start from pairwise similarity and have several approach:

1. *single linkage*: minimum distance between units belonging to different cluster (least distant couple)

2. *complete linkage*: maximum distance between units belonging to different cluster (most distant couple of units)

3. agerage linkage: mean distance between units belonging to different cluster (compromise of the two above)

Remark 12. The previous methods works for *any variable* (eg we can apply Jaccard, Gower and so on to calculate the distances between units/groups).

Among the agglomerative methods there are two more options that works for *numerical variables only*:

1. centroid methods

2. Ward's methods

Important remark 11. In case in, if in the distance matrix we have two *identical minimum distances*, we toss a coin to choose which one to aggregate.

2.3.1 Single linkage

Having two groups C and G their distance is the minimum distance between the units

$$d_{CG} = \min_{j \in C, h \in G} d_{jh}$$

single linkage is also known as *nearest neighbor*. Thus one has to compute all the pairwise distances between all the units in the first and the second group: then the distance between the groups is the distance between the closest point belonging to the different groups.

Example 2.3.1. Assume we have thid distance matrix D between units of our sample (a, b, c, e) per il momento indico in questo modo la matrice facendo riferimento alle unità ...

$$\mathbf{D} = \begin{bmatrix} & a & b & c & e \\ a & 0 & 1 & 4 & 3 \\ b & & 0 & 2 & 7 \\ c & & & 0 & 5 \\ e & & & & 0 \end{bmatrix}$$

To cluster this dataset using single link we start by putting together the closest units: a and b are the two most similar which have **distance 1**. To update the distance matrix and re-iterate, we apply the single linkage definition to calculate the distance of these groups. We obtain

$$\mathbf{D} = \begin{bmatrix} & (a, b) & c & e \\ (a, b) & 0 & 2 & 3 \\ c & & 0 & 5 \\ e & & & 0 \end{bmatrix}$$

where the elements of the new first row (the only changing) were calculated as

$$d_{(a,b),c} = \min(d_{ac}, d_{bc}) = \min(4, 2) = 2$$
$$d_{(a,b),e} = \min(d_{ae}, d_{be}) = \min(3, 7) = 3$$

Now we iterate and choose to aggregate the group with the minimum distance which are (a, b) and c with **distance 2**. The new distance will be

$$\mathbf{D} = \begin{bmatrix} & (a, b, c) & e \\ (a, b, c) & 0 & 3 \\ e & & 0 \end{bmatrix}$$

where we obtained

$$d_{(a,b,c),e} = \min(d_{ae}, d_{be}, d_{ce}) = \min(3, 5, 7) = 3$$

So the final distance between the units will be **3**.
To build the dendogram, we put units on the x axis and distances on which are grouped on the y axis

TODO: figura dendogramma lezione 3, primo esempio

This is clustering obtained with single linkage: risk of this method is to obtain strange groups since has the tendency to put togheter heterogenous units. This because single linkage is affected by *chaining effect*: assume that we have two groups because the near two YELLOW ighlighet points the two groups tend to be put togheter (in subsequent iterations)

TODO: seconda immagine

It has the advantage of being flexible

2.3.2 Complete linkage

Also called *farthest neighbors*, the distance between groups is defined as

$$d_{CM} = \max_{j \in C, h \in G} d_{jh}$$

Example 2.3.2. Starting from the very same matrix of differences

$$\mathbf{D} = \begin{bmatrix} & a & b & c & e \\ a & 0 & 1 & 4 & 3 \\ b & & 0 & 2 & 7 \\ c & & & 0 & 5 \\ e & & & & 0 \end{bmatrix}$$

we put together the most similar units, so a, b (which have **distance 1**); the only change is in how we calculate the distance between groups and update the distance matrix

$$\mathbf{D} = \begin{bmatrix} & (a,b) & c & e \\ (a,b) & 0 & 4 & 7 \\ c & & 0 & 5 \\ e & & & 0 \end{bmatrix}$$

where we calculated

$$\begin{aligned} d_{(a,b),c} &= \max d_{ac}, d_{bc} = \max 4, 2 = 4 \\ d_{(a,b),e} &= \max d_{ae}, d_{be} = \max 3, 7 = 7 \end{aligned}$$

Now to aggregate I look for the smallest value, which as before (not always the case, btw) are between (a, b) and c with **distance 4**. We construct the final matrix as

$$\mathbf{D} = \begin{bmatrix} & (a,b,c) & e \\ (a,b,c) & 0 & 7 \\ e & & 0 \end{bmatrix}$$

where

$$d_{(a,b,c),e} = \max d_{ae}, d_{be}, d_{ce} = \max 3, 5, 7 = 7$$

So finally we put all the units together with **distance 7**.

TODO: dendogram

Complete linkage tends to produce *spherical grops*: it splits data into balls when we have big jump it means that we're trying to put together groups which are more different

2.3.3 Average linkage

The distance between groups is calculated as:

$$d_{CG} = \frac{\sum_{j \in C, h \in G} d_{jh}}{n_c \cdot n_g}$$

where at the denominator we have all the comparison between units of the two groups.

Example 2.3.3. Starting from the very same matrix

$$\mathbf{D} = \begin{bmatrix} & a & b & c & e \\ a & 0 & 1 & 4 & 3 \\ b & & 0 & 2 & 7 \\ c & & & 0 & 5 \\ e & & & & 0 \end{bmatrix}$$

After the first aggregation

$$\mathbf{D} = \begin{bmatrix} & (a,b) & c & e \\ (a,b) & 0 & 3 & 5 \\ c & & 0 & 5 \\ e & & & 0 \end{bmatrix}$$

where we obtained

$$d_{(a,b),c} = \frac{1}{2 \cdot 1}(4+2) = 3$$
$$d_{(a,b),e} = \frac{1}{2 \cdot 1}(3+7) = 5$$

The second step is to merge unit c with group (a,b) (having **distance 3**) obtaining

$$\mathbf{D} = \begin{bmatrix} & (a,b,c) & e \\ (a,b,c) & 0 & 5 \\ e & & 0 \end{bmatrix}$$

where

$$d_{(a,cb,c),e} = \frac{1}{3 \cdot 1}(3+7+5) = 5$$

The final one put together the remaining, having distance 5

TODO: dendrogram

2.3.4 Centroid methods

This and the following methods are for numeric variables only.

$$d_{CG} = \|\overline{\mathbf{x}_C} - \overline{\mathbf{x}_G}\|$$

where $\overline{\mathbf{x}_C}$ is the mean vector of c and $\overline{\mathbf{x}_G}$ is the mean vector of G, That is these are the mid points of the cloud of points associated to a given group in the space. and the distance between them is the distance between the cluster they represent.

Remark 13. Obviously we need numeric variables only to compute the mean vectors; in principle we would need to compute Lance willians formula linkage method
two statistic ian put all the clustering methods in a general family and changing parameter gives us. This is way the centroid put together

TODO: riascolterei qui

2.3.5 Ward's method

Still included in Lance-Williamms, this is the agglomerative analog of Edward-Cavalli-Sforza divisive method. It's based on the decomposition of total sum of square in the within and between components

- We start assuming n cluster each composed by 1 unit: thus our within group sum of WSS=0 (single unit identical to themselves)
- The merging units to groups causes an increase in WSS: so at each step we perform the merge that causes the smallest increase in WSS (create groups which are most similar)

Some remarks:

- since we work with sum of square it's obvious that we need numerical variables
- this was the first method proposed in statistical literature
- has have no strong math properties but they're very populare.

the drawbacks is that

- the cluser they find is localy obtimal (stepwise): if one cut the dendogram at one point and find 5 groups, is not necessarily the best partition overall. it's the best given the steps performed before, all the below in terms of dendrogram, but not necessarily minimize the WSS
- can be slow

TODO: Riascolta $X^T X$ $(m + 1m + 1)$ rank

2.4 Partitioning methods (k-means)

The aim is to provide a single-step partition in k-groups: it's not an hierarchy anymore, its a flat partition.
The most famous methods is the k-means clustering (so as the name says the methods *works for numerics variable only*).

2.4.1 k-means clustering

We want to obtain the partition in k groups, with k given, having the smallest WSS; having our dataset and considered a given k eg $k = 3$. One of the methods (not the unique) with which to implement k-means is the following

```
|----------------------| x <- consider first three rows
|----------------------| x <- of our dataset
|----------------------| x <- as starting centres
|----------------------|
...
|----------------------|
|----------------------|
```

The algorithm start choosing the first three rows in the dataset and consider them as centers of the $k = 3$ groups we want. Then

- i start reading my data matrix and assign the fourth unit to the center to which it is closer. eg i assign unit 4 to the second center
- i compute the center again and I continue reading the matrix in the same way, recomputing the centres after each assignment
- once processed all the dataset and having computed three centers, we start reading again the dataset and reassign all the observation to the nearest center of the three

This method is also known as dynamic cloud because every time a unit is added the cloud, its cloud/means moves (and the centre as well)

So:

- The method we've seen depends on the first three units, for this reason we make a second passage/run in the dataset. The first is to find reasonable centers, the second is to find the groups starting from reasonable centers/to produce the final assingment.
- seems time consuming but it's faster than hierarchical methods. (procedure is called fast clust in SAS) and allows to analyze a large number of units at the same time

Remark 14. Problem with k-means is that one has to chose k in advance: we have to have a criterion how many groups to choose,

2.4.2 Other methods like k-means

Before continuing with k-means we briefly mention two methods which are becoming more and more popular in clustering literature.

2.4.2.1 PAM

Very popular method and close to k-means, PAM[1] stands Partitioning Around Medoids: what a medoid is? it's a prototypical unit. It is an observed unit: as opposite to k-means (where the means doenst correspond to a real object) the medoid is a real observation which act as center. The goal is to find the unit that best represents the groups in the unit; the medoid can be taken as example idea close to k-means but the center is a real unit not a mean of observations algorithmically it becomes more complicate than k-means. This allow to work with non numeric variables we use any distance that we'veseen and find the unit which minimise that distances. Same strategy as k-means as it is a partitioning method but the group centers must be observed units. It can be used with any kind of data while k-means assumes numeric variables only

[1]Peter Rousseaw has invented this method and created the Rousseaw prize (nobel prize for statistics) First winner were research harvard on causal inference. Second those the FALSE discovery rates (benjamini hochberg)

2.4.2.2 Model based clustering

All methods seen so far are distribution free: we made no assumption regarding probability distribution that generated the data.
On the other hand if we can rely on probabilistic assumptions there's a big family of method, the *model based clustering*, which rely on the hypothesis that data are generated by a probabilistic model.
Idea is not new (Pearson did it in univariate case): assume we want study height, so X is height $F(x)$ is pdf of height. After having obtained and seen the data we can imagine that height of the group is generated by sampling from a probability density.
But the point is that in this group there're males and females; so overall F probability seen is a mixture of two probability functions/density, from males and density of females.

$$F(x) = \pi_m F_m(x) + \pi_f F_f(x)$$

π_m and π_f are proportion of males and females proportions so it is assume to be $\pi_m + \pi_f = 1$ in the population. π_m, π_f are known as *mixing proportion.*
Now I can make assumption

$$F_m(X) \sim N(mu_m, sigma_m^2)$$
$$F_f(X) \sim N(mu_f, sigma_f^2)$$

I can rewrite my $F(x)$ as

$$F(x) = \pi_m \phi(x, mu_m, sigma_m^2) + \pi_f \phi(x, mu_m, sigma_m^2)$$

where ϕ is probabilty density function of normal distribution computed in x with mean and variace coming from the two population.
This above is called a *finite mixture model*: in order to obtain the observed and unknown $F(x)$ we need to work on the component μ_m, μ_f (while π_m and π_f are still the mixting proportion). We have to guess the πs and μs.
Pearson started from a simpler case: I *know* the mixing proportions πs, and assume that the shape of my component densities is Gaussian. My problem is to estimate the parameters of the normal distribution which gives me the $F(x)$ that best fit my data. Starting from this idea people have tried to complicate the problem:

- first assuming we don't know the mixing proportion. This can be overcome with different attempt using different mixing proportions
- not knowing the number of cluster
- extending to multiple variables: here we need to estimate mean vector and covariance matrices as well (not single mean and variances). It took a while but recently people invented methods to estimate EM algorithm

TODO: CHECK this 17/2

$$F(\underline{\mathbf{x}}) = \sum_{g=1}^{G} \pi_g \cdot F_g(\underline{\mathbf{x}})$$

with priori probability of group membership $\sum_{g=1}^{G} pi_g = 1$ and F_g groups specific density functions. In the case of gaussian components

$$F(\underline{\mathbf{x}}) = \sum_{g=1}^{G} \pi_g \cdot \phi(\underline{\mathbf{x}}, \mu_g, \Sigma_g)$$

and this is called gaussian mixture models (GMM).
A priori we dont' have number of groups but we have the likelihood to guide us to estimate to select good value for parametrs.
k-means has been proved to be one particular case of these model where variables are uncorrelated and have the same variance (variance covariance matrix is diagonal).
Other methods have been proposed which are not based on gaussian (mixture of multivariate T, and so on).

2.4.3 Choice of k in k-means

Back to k-means, problem with it is that we need to specify k in advance but in many application we don't know the number of groups. So we need criteria:

- what's the most reasonable value for k
- i've partitioned into k groups is good or bad? $k + 1$ is better?

we need to measure quality of clustering: a couple of idea/two different measures

2.4.3.1 Silhouette score

Average silhouette width (by Peter Rousseau, quello del nobel per la statistica), once obtained the clustering, is based on two ingredients:

- $a(j)$ is the average dissimilarity between unit j and the other units onging to the same group
- $b(j)$ average dissimilarity between unit j and the units that belong to the closest group to the one unit j belongs (so I calculate the distabnces between the unit j and all the otgher units in all the other and choose the best group other than that where the unit is assigned)

Then i can calculate the *silhouette of a unit*, defined as **TODO**: CHECK 17/2

$$s(j) = \frac{b(j) - a(j)}{\max[a(j), b(j)]}$$

where we compare the distance of units to that of the most near other group.
I expect that the numerator is positive (more similar to the groups it belongs to respect to other), then I normalize the quantity by considering the max value.
This quantity can go from -1 to +1:

- +1 means that units have been perfectly assigned
- 0 means taht it could be assigned equally to the group who belong or the group with more similar units (in some sense assignment done by clustering is neutral, one group or the other is teh same)

- -1 means wrong sasignment: the unit is more similar to the other group respect to the group who were assigned. the second best group wold have been better

TODO: graph

Example 2.4.1. In the example the silhouette of x_1

$$a(x_1) = \frac{3+5}{2} = 4$$
$$b(x_1) = \min\left(\frac{6+8}{2}, \frac{10+12}{2}\right) = 7$$
$$s(x_1) = \frac{7-4}{7} = \frac{3}{7}$$

So if $s(j)$ is larger than 0, as in this case, than this is good assignment.

Finally to measure the quality of clustering we compute the average silhouette

$$\bar{s} = \frac{\sum_{j=1}^{n} s(j)}{n}$$

some units will be correclty classified, some neutral some badly classified so we expect that the clustering is better if **s** is near to 1. So in general the higher the mean better and good clustering quality is obtained when $\bar{s}$ is close to 1.
Drawback of this approach: here we have to have at least two groups, so this method does not allow to check if actually the best k is 1, that is it doesn't allow to check the actual existence of different groups.
Finally silhouette are plotted in the silhouette plot: graph of the silhouette profile of each individual is reported and coloring according to the group (meaningful if we have few units)

Pearson's gamma

Another measure of clustering quality is known as Pearson's γ: this is nothing but a linear correlation coefficient r, computed on special things

All the cluster we've considered put together a,b,c and let e alone. To compute Pearson's gamma (single linkage example) starting from the original dissimilarity matrix TODOHERE

$$\mathbf{D} = \begin{bmatrix} & a & b & c & e \\ a & 0 & 1 & 4 & 3 \\ b & & 0 & 2 & 7 \\ c & & & 0 & 5 \\ e & & & & 0 \end{bmatrix}$$

First we "vectorize" it putting all upper triangular distances (outside diagonal) in vector form and add a dummy vector/variable which takes value 1 if units are assigned to different group after clustering, 0 otherwise

$$d = \begin{bmatrix} d_{ab} \\ d_{ac} \\ d_{ae} \\ d_{bc} \\ d_{be} \\ d_{ce} \end{bmatrix} = \begin{bmatrix} 1 \\ 4 \\ 3 \\ 2 \\ 7 \\ 5 \end{bmatrix}, \quad g = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \end{bmatrix}$$

In the final clustering we had we had a, b, c and e alone; above in g is reported the corresponding vector.

Pearson's γ is just the correlation coefficient between d and g (between the distance and the fact that units are assigned to different groups or the same group

$$\gamma = frac \sum_{i=1}^{n(n-1)/2} d_i g_i - \frac{n(n-1)}{2}\overline{dg} \sqrt{\sum_{i=1}^{n(n-1)/2} d_i^2 - \frac{n(n-1)}{2}\overline{d}^2} \sqrt{\sum_{i=1}^{n(n-1)/2} g_i^2 - \frac{n(n-1)}{2}\overline{g}^2}$$
$$= \frac{codev(d, f)}{\sqrt{dev(d)dev(g)}}$$

the sum is on i which are the number of unique elements out of the diagonal. The measure is a correlation which take range between -1 and 1:

TODO: CHECK 17/2

- large positive values close to +1 means that distant units tend to be clustered in different group and close units tend to be clustered together
- values close to 0 means that the classification is almost random
- negative values mean that the classification is a mess: we have put in the same group different units and put in different groups similar units.

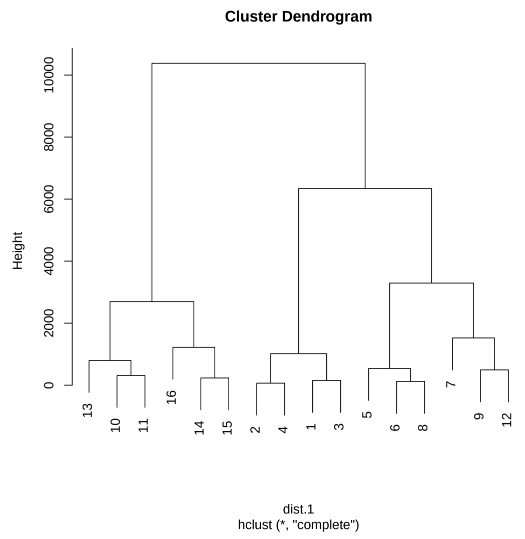
So again as before the larger the better: good clustering correspond to large positive values for γ.

2.5 Lab

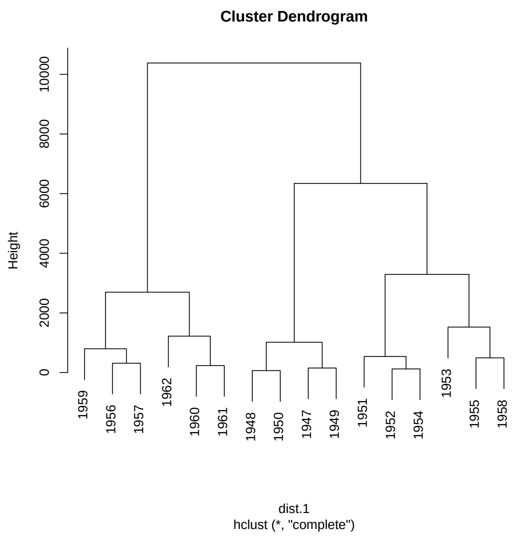
```
## we start by finding distance matrixes among observation
(data <- read.table("data/data.txt", header = TRUE))

##   Att.1 Att.2 Att.3 Att.4 Att.5 Att.6
## 1     1     1     1     0     0     1
## 2     1     0     0     1     0     1
## 3     1     0     0     1     0     1
## 4     0     0     0     0     1     0

## dataset with just binary variables (attributes present or not)
## in situation like this a common distance is jaccard: we compute it using
## dist function (euclidean distance done by default)
dist(data, method = "binary") # it computes lower triangular (symmetric)

##     1   2   3
## 2 0.6
## 3 0.6 0.0
## 4 1.0 1.0 1.0
```

```
# mixed-type data:
library(cluster)
data(flower)
head(flower) # ?flower:

##   V1 V2 V3 V4 V5 V6  V7 V8
## 1  0  1  1  4  3 15  25 15
## 2  1  0  0  2  1  3 150 50
## 3  0  1  0  3  3  1 150 50
## 4  0  0  1  4  2 16 125 50
## 5  0  1  0  5  2  2  20 15
## 6  0  1  0  4  3 12  50 40

# first three binary (third is asimmetric binary), fourth/fifth categorical,
# 6th/7th quantitative

## with this kind of data, the gower distance: in R the function implementing
## it is called daisy: see ?daisy

## we tell daisy the third
gower <- daisy(flower,
               metric = 'gower',
               type = list(asymm = 3)) # treat third is asymmetric binary

## better to check
summary(gower)

## 153 dissimilarities, summarized :
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##  0.1418  0.4164  0.5101  0.5098  0.6051  0.8875
## Metric :  mixed ;  Types = N, N, A, N, O, O, I, I
## Number of objects : 18

## we have
## two N: nominal,
## one A: asymmetric
## two O: ordered factor,
## two I: numeric,

## back to dichotomic data let's see the longley dataset
# install.packages("AER")
library(AER)

## Caricamento del pacchetto richiesto:  car
## Caricamento del pacchetto richiesto:  carData
##
## Caricamento pacchetto:  'car'
## Il seguente oggetto è mascherato da 'package:lbmisc':
##
##     recode
## Caricamento del pacchetto richiesto:  lmtest
## Caricamento del pacchetto richiesto:  zoo
##
## Caricamento pacchetto:  'zoo'
## I seguenti oggetti sono mascherati da 'package:base':
##
##     as.Date, as.Date.numeric
## Caricamento del pacchetto richiesto:  sandwich
## Caricamento del pacchetto richiesto:  survival
```

```
data(Longley) # ?Longley: time series, observation are years
## we want to look employment: we need to extract it from the ts
longley <- as.data.frame(Longley)
X <- longley$employment  ## employment is numeric (for regarding distances)
labels.X <- as.character(1947:1962)    ## name of the years

## now find the distance: different distance can be used (most used is euclidean)
dist.1 <- dist(X, method = 'euclidean')
dist.2 <- dist(X, method = 'manhattan')

## we start clustering with hierarchical methods: ?hclust takes as input the
## dissimilarity and then we specify the method

h <- hclust(dist.1) # "complete" linkage (by default) on euclidian distance h
plot(h) # the dendrogram, without rownames it's a mess
```



```
plot(h, labels = labels.X) # much better
```



```
## how the tree was built during time?
h$merge
```

```
##       [,1] [,2]
##  [1,]   -2   -4
##  [2,]   -6   -8
##  [3,]   -1   -3
##  [4,]  -14  -15
##  [5,]  -10  -11
##  [6,]   -9  -12
##  [7,]   -5    2
##  [8,]  -13    5
##  [9,]    1    3
## [10,]  -16    4
## [11,]   -7    6
## [12,]    8   10
## [13,]    7   11
## [14,]    9   13
## [15,]   12   14
```

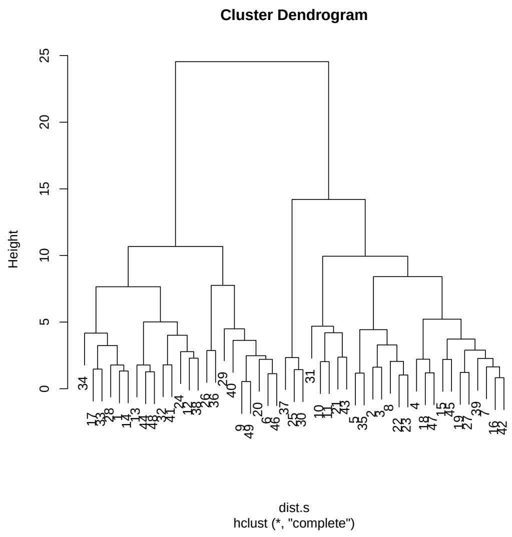
```
## a matrix with two columns:
## to understand this look at the first with id
## 1) starting from the first row: the dendrogram is built bottom to top
## when we have two negative values (-2 and -4) the observation are merged
## together
## 2) in row 7 a negative and a positive value: the observation with negative
## sign has been merged with cluster built at step said by column: so unit 5
## was ## merged with cluster at row 2, so with observation 6 and 8
## 3) both positive values: 1 and 3 in row 9. Cluster formed in row 1 (2 and 4)
## has been merged with row 3 (observation 1 and 3)

## height is important: look at distances between
```

```
h$height

##  [1]    65   122   152   233   312   494   540   798  1016  1220  1524  2694
## [13]  3292  6342 10380

h.cl = c() # empty vector
h.cl[1] = h$height[1] # difference between height at the second step and first
for (i in 2:length(h$height)){
  h.cl[i] = h$height[i] - h$height[i-1]
}

## h.cl now contains differences between useful to cut the tree: we cut at the
## max distance which.max(h.cl) # the largest difference was obtained in the
## last step

## now we need to extract the height to which it correspond the maximum
## distance h.max <- h$height[ which.max(h.cl) -1 ] # we want to cut the tree
## before the max distance so -1 is needed

## final
plot(h, labels = labels.X)
abline(h = h.max, col = "red")

## Error:  oggetto 'h.max' non trovato

## with complete linkage the best number of group is two
## we extract the classification with cutree

cl <- cutree(tree = h, k = 2) # cut to create two groups
cl

##  [1] 1 1 1 1 1 1 1 1 1 2 2 1 2 2 2 2

cl <- cutree(tree = h, h = h.max) # cut using an height: the h.max

## Error:  oggetto 'h.max' non trovato

## this was complete linkage: other methods one has only to change methods at
## the beginning.

h <- hclust(dist.1, method = "average")

## and then all the code is equal (results may be different) with average
## linkage the best number of group is still 2
```

I had problems with pc, look at scripts uploaded (al back to normal with k-means)

```
## another dataset

head(sparrow <- read.table("data/sparrows.dat", header = TRUE))
```

```
##   totL AlarE  bhL   hL   kL
## 1  156   245 31.6 18.5 20.5
## 2  154   240 30.4 17.9 19.6
## 3  153   240 31.0 18.4 20.6
## 4  153   236 30.9 17.7 20.2
## 5  155   243 31.5 18.6 20.3
## 6  163   247 32.0 19.0 20.9

## dataset about sparrow during a storm: some of them died while some other
## survived (we don't know if they died or survived in the dataset): the died
## are from row 22 to 49 btw

## we want to see if clustering these observation we found a link between their
## death and characteristics
## again all numeric

dist.s = dist(sparrow, method = 'euclidean')

h <- hclust(dist.s) # "complete" linkage (by default) on euclidian distance h
plot(h) # the dendrogram, without rownames it's a mess
```



```
## how the tree was built during time?
h$merge # a matrix with two columns:

##       [,1] [,2]
##  [1,]   -9  -49
##  [2,]  -16  -42
##  [3,]  -22  -23
##  [4,]   -6  -46
##  [5,]   -5  -35
##  [6,]  -18  -47
##  [7,]  -19  -27
##  [8,]  -44  -48
##  [9,]   -1  -14
## [10,]  -25  -30
## [11,]  -17  -33
## [12,]   -2   -3
## [13,]   -7    2
## [14,]  -28    9
## [15,]  -13    8
## [16,]  -32  -41
## [17,]  -10  -11
## [18,]   -8    3
## [19,]  -15  -45
## [20,]  -20    4
## [21,]   -4    6
## [22,]  -39   13
## [23,]  -12  -38
## [24,]  -37   10
## [25,]  -21  -43
## [26,]    1   20
## [27,]  -24   23
## [28,]  -26  -36
## [29,]    7   22
## [30,]   11   14
## [31,]   12   18
## [32,]  -40   26
## [33,]   19   29
## [34,]   16   27
## [35,]  -34   30
## [36,]   17   25
## [37,]    5   31
## [38,]  -29   32
## [39,]  -31   36
## [40,]   15   34
## [41,]   21   33
## [42,]   35   40
## [43,]   28   38
## [44,]   37   41
## [45,]   39   44
## [46,]   42   43
## [47,]   24   45
## [48,]   46   47
## to understand this look at the first with id

## 1) starting from the first row: the dendrogram is built bottom to top when
## we have two negative values (-2 and -4) the observation are merged together

## 2) in row 7 a negative and apositive value: the observation with negative
## sign has been merged with cluster built at step said by column: so unit 5
## was merged with cluster at row 2, so with observation 6 and 8
## 3) both positive values: 1 and 3 in row 9. Cluster formed in row 1 (2 and 4)
## ## has been merged with row 3 (observation 1 and 3)

## height is important: look at distances between h$height
h.cl = c() # empty vector
h.cl[1] = h$height[1] # difference between height at the second step and first
for (i in 2:length(h$height)){
  h.cl[i] = h$height[i] - h$height[i-1]
}

## h.cl now contains differences between useful to cut the tree: we cut at the
## max distance
which.max(h.cl) # the largest difference was obtained in the last step

## [1] 48

## now we need to extract the height to which it correspond the maximum
## distance
h.max <- h$height[ which.max(h.cl) -1 ] # we want to cut the tree before the
                                        # max distance so -1 is needed

## final
plot(h, labels = labels.X)
```

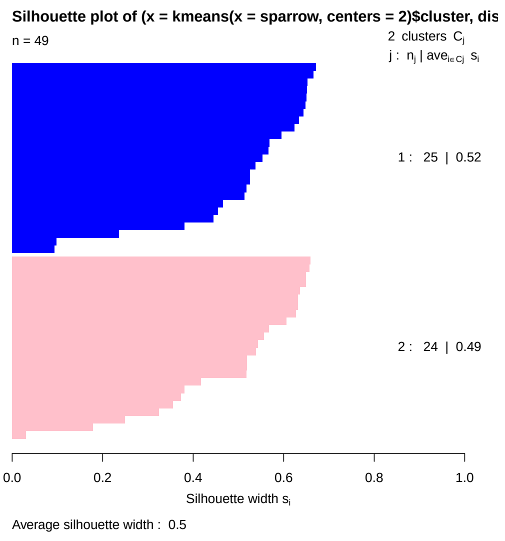
```
## Error in graphics:::plotHclust(n1, merge, height, order(x$order),
hang, :  dendrogramma in input non valido

abline(h = h.max, col = "red")
## with complete linkage the best number of group is two we extract the
## classification with cutree
```

```
cl <- cutree(tree = h, k = 2) # cut to create two groups cl # first assigned tofirst group
cl <- cutree(tree = h, h = h.max) # cut using an height: the h.max
```

the methods agrees that best method in hierarchical clustering is 2

2.6 K-means

```
set.seed(1234) ## if we run this function we could get different results, set the seed
km <- kmeans(x = sparrow, centers = 2) # x is the data, we start with two groups

## extract the cluster k-means built
km$cluster # info on clusters: there's not a link between clustering and the

##  [1] 1 2 2 2 2 1 2 2 1 2 2 1 1 1 2 2 1 2 2 1 2 2 2 1 2 1 2 1 1 2 1 1 1 1 2 1 2 1
## [39] 2 1 1 2 2 1 2 1 2 1 1

# actual dead: (dead are the last one)
km$centers # info on centroids

##       totL    AlarE      bhL       hL       kL
## 1 160.9167 245.4583 31.90417 18.80833 21.29583
## 2 155.1600 237.3600 31.03200 18.14400 20.37600

## supposing we dont' know the number of groups: we have to chose it in some
## way

## install.packages("fpc")
library(fpc)

## average silhouette and pearson gamma for several n of k groups
## build a matrix of

indexes <- matrix(NA, nrow = 5, ncol = 2)
for (k in 2:5){
  set.seed(1234)
  km <- kmeans(x = sparrow, centers = k) # centers = k
  stats <- cluster.stats(dist.s, # distance as first object, clustering as second
                         km$cluster)
  indexes[k, ] <- c(
    stats$avg.silwidth, ## average silhouette width in first col
    stats$pearsongamma   ## average pearson gamma second col
  )
}

indexes

##           [,1]      [,2]
## [1,]        NA        NA
## [2,] 0.5046398 0.6496322
## [3,] 0.3375809 0.5476798
## [4,] 0.3925813 0.6049124
## [5,] 0.3952145 0.5493019

## we need to look by column: maximum value for both indicator is k=2 (at least
## with this seed). both indexes agree

## plot silhouette of the two groups
library(cluster)
silhouette

## function (x, ...)
## UseMethod("silhouette")
## <bytecode: 0x559bb909cb78>
## <environment: namespace:cluster>

## silhouette
sil <- silhouette(kmeans(x = sparrow, centers = 2)$cluster,
                  dist.s
                  ) # x is the clustering for the best
plot(sil, col = c("blue", "pink"))
```



```
# silhouette width of eachobservation
```

Capitolo 3

Principal component analysis

With qualitative data correspondence analysis to do the same shit

3.1 Linear combinations

Definition 3.1.1 (Linear combination)**.** A linear combination is sum of vector with weights given from another vector. Assuming we have a random vector X including p random variables (dimension $p \times 1$) a and a vector of constant terms:

$$\underset{p\times 1}{\mathbf{x}} = \begin{bmatrix} X_1 \\ \dots \\ X_i \\ \dots \\ X_p \end{bmatrix}, \quad \mathbf{a} = \begin{bmatrix} a_1 \\ \dots \\ a_i \\ \dots \\ a_p \end{bmatrix} \in \mathbb{R}^p$$

a linear combination Y of the two is

$$Y = \mathbf{a}^\top \mathbf{x} = a_1 X_1 + \ldots + a_i X_i + \ldots a_p X_p$$

We have that Y is a linear combination of the random variables in $\mathbf{x}$ with weights given by the components/coefficients of $\mathbf{a}$; Y is a scalar random variable (has dimension 1×1).

Important remark 12. We assume that:

- our random vector $\mathbf{x}$ has expected value/means $\mathbb{E}[x] = \boldsymbol{\mu}$: each X_i has its own expected values and we collect all these expected value in a vector

$$\mathbb{E}[\mathbf{x}] = \boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \dots \\ \mu_i \\ \dots \\ \mu_p \end{bmatrix} = \begin{bmatrix} \mathbb{E}[X_1] \\ \dots \\ \mathbb{E}[X_i] \\ \dots \\ \mathbb{E}[X_p] \end{bmatrix}$$

- our vector $\mathbf{x}$ has covariance matrix denoted by $\boldsymbol{\Sigma}$ which is a $p \times p$ matrix with variances on the diagonal and covariances out of the diagonal. Since it's square and symmetric for simplicity people just report the upper matrix:

$$\operatorname{Var}[X] = \underset{p\times p}{\boldsymbol{\Sigma}} = \begin{bmatrix} \sigma_1^2 & \dots & \sigma_{1i} & \dots & \sigma_{1p} \\ & & \sigma_i^2 & \dots & \sigma_{ip} \\ & & & & \sigma_p^2 \end{bmatrix}$$

3.1.1 Variance of linear combinations

Important remark 13. What happens to expected value and variance/covariance if we take a linear combination of the variable:

- for the expected value we have

  $$\mathbb{E}[Y] = \mathbb{E}\left[\mathbf{a}^\top \mathbf{x}\right] = a^\top \mathbb{E}[\mathbf{x}] = \mathbf{a}^\top \boldsymbol{\mu} = a_1\mu_1 + \ldots + a_i\mu_i + \ldots + a_p\mu_p$$

  so the expected value of a linear combination is the linear combination of the expected values (and is a scalar)

- regarding the variance, to obtain the analog of the square we have to multiply pre and post for $\mathbf{a}$ respecting dimensions

  $$\operatorname{Var}[Y] = \operatorname{Var}\left[\mathbf{a}^\top \mathbf{x}\right] \overset{(1)}{=} \underset{1\times p}{\mathbf{a}^\top} \underset{p\times p}{\operatorname{Var}[\mathbf{x}]} \underset{p\times 1}{\mathbf{a}} = \underbrace{\mathbf{a}^\top \boldsymbol{\Sigma} \mathbf{a}}_{1\times 1}$$

  where in (1) we used the equivalent of $\operatorname{Var}[aX] = a^2 \operatorname{Var}[X]$ in case of random vector instead of single variable. So the variance is a scalar as well

Considering the simple case of $\mathbf{x}$ composed by two variable $\mathbf{x} = [X_1, X_2]^\top$, this means that

$$\begin{aligned} \operatorname{Var}[Y] = \mathbf{a}^\top \boldsymbol{\Sigma} \mathbf{a} &= \begin{bmatrix} a_1 & a_2 \end{bmatrix} \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \\ &= \begin{bmatrix} a_1\sigma_1^2 + a_2\sigma_{12} & a_1\sigma_{12} + a_2\sigma_2^2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \\ &= a_1^2 + \sigma_1^2 + a_1a_2\sigma_{12} + a_1a_2\sigma_{12} + a_2^2\sigma_2^2 \\ &= a_1^2\sigma_1^2 + 2a_1a_2\sigma_{12} + a_2^2\sigma_2^2 \end{aligned}$$

Focusing

- on the first element a_1 thinking variance as function of a_1 what happens to the variance when a_1 changes? This is an upward parabola (coefficient σ_1^2 is necessarily positive being a variance) : as a_1 varies the variance describe an upward parabola
- focusing on a_2 it's the same thing, again it's an upward parabola

In our bidimensional space, variance as fuction of a_1, a_2 (taken as x, y) is a cup: the variance goes to infinity, does not have a finite maximum. We can increase the variance of linear combination just by simply increasing the value of a_1 and a_2

In other words, in the multidimensional space the variance of a linear combination can be increased just by using a vector $\mathbf{a}$ with larger norm: the larger the norm of the vector $\mathbf{a} = (a_1, a_2)$ the larger the variance of the linear combination it produces.
So the variance of a linear combination does not have a finite maximum. Keeping the data as fixed we can increase the variance of a linear combination by simply increasing the norm of the vector a containing coefficient of the linear combination $\mathbf{a}$
This is something we don't like: we want something that is linked to the data for an increase in variance. This is a point important for principal component.

Important remark 14. To take the linear algebra approach the variance $\mathrm{Var}[Y] = \mathbf{a}^\top \Sigma \mathbf{a}$ is a quadratic form, represented by a positive semidefinite matrix.
So a positive semidefinite quadratic form does not have a finite maximum.

Remark 15. These are two different way of saying the same and are the preliminaries for PCA.

3.1.2 Multiple linear combinations

Remark 16. We have more than 1 linear combinations: in that case we can collect the weights in a matrix called $\boldsymbol{A}$, that will be a $p \times q$ where q is the number of linear combinations we're interested in.[1]

Important remark 15. A vector of q linear combinations $\mathbf{y}$ $(q \times 1)$ can be obtained as

$$\underset{q\times 1}{\mathbf{y}} = \underset{q\times p}{\mathbf{A}^\top} \underset{p\times 1}{\mathbf{x}}$$

Properties of mean and variance of transformations applies again so:

$$\mathbb{E}[Y] = \mathbf{A}^\top \mathbb{E}[X] = \mathbf{A}^\top \boldsymbol{\mu}$$
$$\mathrm{Var}[Y] = \mathbf{A}^\top \mathrm{Var}[X]\,\mathbf{A} = \mathbf{A}^\top \boldsymbol{\Sigma} \mathbf{A}$$

with $\mathbb{E}[Y]$ a $q \times 1$ vector and $\mathrm{Var}[Y]$ no longer a scalar but a $q \times q$ matrix (Since we have more than one random variable there is not only the variances but also the covariances).

Example 3.1.1. Assume we have a bivariate random vector $\mathbf{x} = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}$ with mean $\boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$ and variance/covariance matrix $\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix}$.
Now let's consider the following linear combinations

$$Y_1 = X_1 - X_2$$
$$Y_2 = X_1 + X_2$$

Derive the expected values and the covariance matrix of $Y = \begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix}$

[1]Warning: we've no enough letters so the notation is consistent within each topic. This matrix $\mathbf{A}$ has to do nothing with the centering matrix seen before. In this chapter $\mathbf{A}$ is the matrix of coefficients

Example 3.1.2. Consider three independent standardized variables Z_1, Z_2, Z_3. Assume we transform them as

$$\begin{aligned} Y_1 &= Z_1 \\ Y_2 &= Y_1 + 0.01 \cdot Z_2 \\ Y_3 &= 10 \cdot Z_3 \end{aligned}$$

derive the covariance matrix of $Y = \begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix}$

3.2 PCA

Principal component analysis has been invented by Pearson in 1901, but the way we'll see it is not based on the development of Hotelling in 1933. They wanted to solve two different problem but found to obtain the same solutions, they've both invented it:

- Pearson wanted to solve a regression problem (1901 "On lines and planes of closest fit to a system of points"); he wanted to find a line that best fit the point, but in a special condition where he had errors in the predictors[2].
- Hotelling OTOH have too many variables and can't find a way to manage them so wanted to summarize them producing a smaller number of variables that keep as much info as in the original sets. Hotelling found a low dimensional function (linear combination) of the observed data that preserves as much of the variability as possible. The approach is the same used at today.

They didn't have machines to do calculations, but used cleverly linear algebra, eigenvalue and eigenvector to tackle the problem.

3.2.1 First principal component

Let's start by considering a single linear combination of the variables (we see other combination afterward); we have

$$y_1 = \mathbf{a}_1^\top \mathbf{x}$$

The point is that we want to find a linear combination (so determines the values of a_1), such that the variance of the combination $\text{Var}[y_1] = \mathbf{a}_1^\top \mathbf{\Sigma} \mathbf{a}_1$ is maximum. Problem is that, as we've seen before, a maximum on variance does not exists: it is enough to take $\mathbf{a}_1$ with norm higher and higher.
What interests us is actually the direction of the vector $\mathbf{a}_1$: in that case I can put a constraint on the norm of $\mathbf{a}_1$ (in other words to have a fair comparison between vectors to find the higher variance, we put a constraint on the norm). In this case a unit norm vector is enough to identify a direction in space, so the constraint that we put is that $\|\mathbf{a}_1\| = 1$, that is $\mathbf{a}_1^\top \mathbf{a}_1 = 1$.
So finally the problem we need to solve is a *constrainted optimization problem.*

[2]While in regression models one assumes that the x's are fixed without errors, Pearson was in a different situation having error in x

That is we want to choose $\mathbf{a}_1$ to maximize $\text{Var}[y_1] = \mathbf{a}_1^\top \boldsymbol{\Sigma} \mathbf{a}_1$ under the constraint $\|\mathbf{a}\| = \mathbf{a}_1^\top \mathbf{a}_1 = 1$.
This can be solved by using Lagrange multiplier; the problem above is equivalent to maximize this function:

$$\phi = \mathbf{a}_1 \boldsymbol{\Sigma} \mathbf{a}_1 - \lambda_1 (\mathbf{a}_1^\top \mathbf{a}_1 - 1)$$

where λ_1 is a Lagrange multiplier.
Now we need to maximize by taking derivatives, $\mathbf{a}_1$ is our unknown; we check/consider all possible unit norm vector, and put a system of p equations (we need to take p different derivatives, one for each element of $\mathbf{a}_1$) where:

$$\frac{\partial \phi}{\partial \mathbf{a}_1} = 2\boldsymbol{\Sigma}\mathbf{a}_1 - 2\lambda_1 \mathbf{a}_1$$

which equaled to $\mathbf{0}$ yields

$$\boldsymbol{\Sigma}\mathbf{a}_1 = \lambda_1 \mathbf{a}_1$$

That is we need to find the $\mathbf{a}_1$ that satisfy the equation above: so *the solution to the problem consist in a pair of eigenvalue-eigenvector* for the matrix $\boldsymbol{\Sigma}$.
This above is the identity relationship between eigenvalues and eigenvectors: this holds if $\mathbf{a}_1$ is eigenvector of $\boldsymbol{\Sigma}$ and λ_1 is the corresponding eigenvalue.
How many eigenvalues has $\boldsymbol{\Sigma}$? p, since it is $p \times p$ so it is expected to have p. Point is that we need just 1: which pair of eigenvalues-vector solves my problem? In order to answer let's premultiply both sides by $\mathbf{a}_1^\top$

TODO: revisit spectral decomposition

$$\begin{aligned}\boldsymbol{\Sigma}\mathbf{a}_1 &= \lambda_1 \mathbf{a}_1 \\ \mathbf{a}_1^\top \Sigma \mathbf{a}_1 &= \lambda_1 \underbrace{\mathbf{a}_1^\top \mathbf{a}_1}_{=1} \\ \mathbf{a}_1^\top \Sigma \mathbf{a}_1 &= \lambda_1\end{aligned}$$

Some points:

- the last one (on the left) is the variance of a linear combination $\mathbf{a}_1 \mathbf{x}$, which correspond to the first eigenvalue. So the eigenvalue coincides with the variance af the linear transformation;
- if we had to choose one, to maximize the variance the quantity on the left, we need to take the largest eigenvalue. So in order to have *maximum variance* we need to consider the *largest eigenvalue* of $\boldsymbol{\Sigma}$ and $\mathbf{a}_1$ will be the corresponding eigenvector.

Definition 3.2.1 (First principal component)**.** The linear combination of having $\mathbf{a}_1$ as vector of coefficients is called *first principal component*:

$$y = \mathbf{a}_1 \mathbf{x}$$

Remark 17. In other words we can say that the first principal component is the linear combination of the observed variables *having the largest variance*. It's variance will be the largest eigenvalue of Σ and the optimal vector of coefficients $\mathbf{a}_1$ will be the corresponding eigenvector.

Remark 18 (Recap). Main point so far:

- principal Components are linear combinations of observed variable: main tool we use is linear combinations.
- any linear combination does not have finite variance; the variance is positive semidefinite ($\mathbf{\Sigma}$) and has no finite maximum. Variance is an upward parabola.
- maximizing without constraint is therefore risky, we could increase fictitiously variance without reference to the data explained. What we're interested in is not the norm of the vector but the direction of the vector; the unit norm is enough to identify direction in space and to make fair comparison we compare vector having the same norm, for simplicity we take unit norm.
- we want to maximize the variance under the constraint looking only at unit norm vectors of combination. We use Lagrange multiplier to do the maximization.
- to find the maximum we take first derivative equal to 0: our function has a maximum because we constraint on a unit norm vector the maximum is reached with eigenvalue/eigenvector equality
- problem is to find suitable pair of eigenvalue eigenvector: which one to consider? the higher, since it is the variance. So we've identified the first principal component

3.2.2 Following components

We've spoken of the first principal components: maybe it's very improbable that a single linear combination is enough and we need more than one.

We've said that $\mathbf{\Sigma}$ has p pairs eigenvalue-eigenvector: with large number of variables it is difficult that a single combination is enough to save all the variability of the higher dimensional space. So we're interested in looking at a second linear combination.
How can we find the second principal component?

- We want the PC to be orthogonal/uncorrelated
- We need to constraint the optimization search in the orthogonal space to what found at the first step

Our second component will be

$$y_2 = \mathbf{a}_2^\top \mathbf{x}$$

with variance

$$\text{Var}\,[y_2] = \mathbf{a}_2^\top \mathbf{\Sigma} \mathbf{a}_2$$

the Lagrange function will be constructed to maximize $\mathbf{a}_2^\top \Sigma \mathbf{a}_2$ under the unit norm constraint $\mathbf{a}_2^\top \mathbf{a}_2 = 1$ and under the constraint that $\mathbf{a}_2$ is orthogonal to $\mathbf{a}_1$, that is $\mathbf{a}_1^\top \mathbf{a}_2 = \mathbf{a}_2^\top \mathbf{a}_1 = 0$. So we obtain:

$$\phi = \mathbf{a}_2^\top \Sigma \mathbf{a}_2 - \lambda_2(\mathbf{a}_2^\top \mathbf{a}_2 - 1) - \lambda_3(\mathbf{a}_1^\top \mathbf{a}_2)$$

above:

- the first constraint to have unit norm in $\mathbf{a}_2$;
- the second is to impose that $\mathbf{a}_1^\top \mathbf{a}_2 = 0$ (we removed -0) so that $\mathbf{a}_1$ and $\mathbf{a}_2$ are orthogonal.

In order to find $\mathbf{a}_2$ we can derive ϕ respect to $\mathbf{a}_2$ which is our unknown

$$\frac{\partial \phi}{\partial \mathbf{a}_2} = 2\boldsymbol{\Sigma}\mathbf{a}_2 - 2\lambda_2\mathbf{a}_2 - \lambda_3\mathbf{a}_1 \tag{3.1}$$

then we set our derivative equal to $\mathbf{0}$. This problem can be simplified a little bit. Let's premultiply both sides by $\mathbf{a}_1^\top$, we have that

$$2\mathbf{a}_1^\top \Sigma \mathbf{a}_2 - 2\lambda_2 \mathbf{a}_1^\top \mathbf{a}_2 - \lambda_3 \underbrace{\mathbf{a}_1^\top \mathbf{a}_1}_{=1} = \mathbf{0} \tag{3.2}$$

Now considering $\mathbf{a}_1^\top \boldsymbol{\Sigma}$ we have

$$\mathbf{a}_1^\top \Sigma = (\Sigma \mathbf{a}_1)^\top = \lambda_1 \mathbf{a}_1^\top$$

so it is related to the first PC. Back to 3.2 we can simplify as

$$\begin{aligned} &2\lambda_1 \underbrace{\mathbf{a}_1^\top \mathbf{a}_2}_{=0} - 2\lambda_2 \underbrace{\mathbf{a}_1^\top \mathbf{a}_2}_{=0} - \lambda_3 \underbrace{\mathbf{a}_1^\top \mathbf{a}_1}_{=1} = 0 \\ &-\lambda_3 = 0 \end{aligned}$$

This implies that $\lambda_3 = 0$. And back to 3.1 this means that therefore the derivative of ϕ with respect to $\mathbf{a}_2$ will be

$$\begin{aligned} &\frac{\partial \phi}{\partial \mathbf{a}_2} = 2\Sigma \mathbf{a}_2 - 2\lambda_2 \mathbf{a}_2 = \mathbf{0} \\ &\boldsymbol{\Sigma}\mathbf{a}_2 = \lambda_2 \mathbf{a}_2 \end{aligned}$$

and this is again an eigenvalue-eigenvector relationship. If we premultiply by $\mathbf{a}_2^\top$

$$\underbrace{\mathbf{a}_2^\top \Sigma \mathbf{a}_2}_{\mathrm{Var}[Y_2]} = \lambda_2 \underbrace{\mathbf{a}_2^\top \mathbf{a}_2}_{=1}$$

so

$$\mathrm{Var}\left[Y_2\right] = \lambda_2$$

as we want the linear combination of $\mathbf{x}$ having the largest variance in the orthogonal complement of $\mathbf{a}_1$ we take λ_2 as the second largest eigenvalue and $\mathbf{a}_2$ will be the corresponding eigenvector.
The second PC is the linear combination of X with $\mathbf{a}_2$ (the eigenvector corresponding to second largest eigenvalue).
Going on this way, for p variables we can find up to p principal components.

3.3 Properties

Having used an orthogonal $\mathbf{a}_2$ we obtain something interesting, PC s have a very relevant statical property.

3.3.1 Uncorrelation of components

Let's consider our:

$$\mathbf{\Sigma a}_2 = \lambda_2 \mathbf{a}_2$$

premultiplying by $\mathbf{a}_1^\top$

$$\mathbf{a}_1^\top \Sigma \mathbf{a}_2 = \lambda_2 \mathbf{a}_1^\top \mathbf{a}_2$$

but we know that for orthogonality constraint $\mathbf{a}_1^\top \mathbf{a}_2 = 0$ so

$$\mathbf{a}_1^\top \mathbf{\Sigma a}_2 = 0$$

what is this? This is the covariance between Y_1 and Y_2, the first two principal components. Let's prove it. Having

$$y_1 = \mathbf{a}_1^\top \mathbf{x}$$
$$y_2 = \mathbf{a}_2^\top \mathbf{x}$$

without loss of generality let's assume for simplicity that $\mathbf{x}$ variables are mean centered. This implies that the covariance between Y_1 and Y_2 is equal to

$$\begin{aligned}\operatorname{Cov}(Y_1, Y_2) &= \mathbb{E}[Y_1 \cdot Y_2] - 0 \\ &= \mathbb{E}\left[\mathbf{a}_1^\top \mathbf{x}\mathbf{x}^\top \mathbf{a}_2\right] = \mathbf{a}_1^\top \mathbb{E}\left[\mathbf{x}\mathbf{x}^\top\right] \mathbf{a}_2 = \mathbf{a}_1^\top \mathbf{\Sigma a}_2\end{aligned}$$

where $\mathbf{x}\mathbf{x}^\top = \mathbf{\Sigma}$ for what seen in statistics.

Remark 19. This means that *principal components are uncorrelated* (covariance is numerator of correlation); first and second principal component are uncorrelated (this is a not scontated gift, under the constraint imposed).
The fact that orthogonal vectors generate uncorrelated variable is not necessarily true: orthogonality and un-correlation are not synonims.[3]

Example 3.3.1. A counterexample. Consider the vectors of the canonic bases

$$\mathbf{e}_1 = \begin{bmatrix}1\\0\end{bmatrix}, \quad \mathbf{e}_2 = \begin{bmatrix}0\\1\end{bmatrix}$$

Any point in $\mathbb{R}^2$ can be obtained as combination of those two.
We're interested in a generic (x_1, x_2) we can think of coordinates as linear combination of vector from canonic base:

$$\begin{bmatrix}x_1\\x_2\end{bmatrix} = x_1\mathbf{e}_1 + x_2\mathbf{e}_2 = \begin{bmatrix}x_1\\0\end{bmatrix} + \begin{bmatrix}0\\x_2\end{bmatrix} = \begin{bmatrix}x_1\\x_2\end{bmatrix}$$

TODO: grafico

Now considering any scatterplot of correlated variable (rugby ball): each point on a cloud of correlated variables X_1 and X_2 can be generated by $\mathbf{e}_1, \mathbf{e}_2$; $\mathbf{e}_1$ and $\mathbf{e}_2$ are orthogonal but the corresponding linear combination are correlated.
The points can be thought of as linear combination with coefficients given by the vectors of the canonical basis (which are orthogonal by definition but the variables are correlated).
On the contrary on PC orthogonal vectors (eigen) and uncorrelated variables.

[3] As an exercise think a counterexample: an example in which you have linear combination of the observed variable that are identified by orthogonal vectors and are correlated

3.4 Obtaining PCs in practice

In practice how to obtain principal components?

$$\begin{aligned}\boldsymbol{\Sigma}\mathbf{a}_1 &= \lambda_1\mathbf{a}_1\\ \boldsymbol{\Sigma}\mathbf{a}_1 - \lambda_1\mathbf{a}_1 &= \mathbf{0}\end{aligned}$$

now we collect $\mathbf{a}_1$ obtaining the identity matrix of the same size

$$(\boldsymbol{\Sigma} - \lambda_1\mathbf{I})\mathbf{a}_1 = \mathbf{0}$$

our problem is to find $\mathbf{a}_1$ which solves this equation.
It's a linear equation system which is homogeneous (constant term is 0): it admits a nontrivial solutions (eg $\mathbf{a}_1 = \mathbf{0}$) the matrix of coefficient needs to be singular, that is its determinant needs to be equal to zero

$$\det(\boldsymbol{\Sigma} - \lambda_1\mathbf{I}) = 0$$

This means that λ_1 should be *a root of the characteristic polinomial.* So finding the principal components amounts to solve eigenvalue/vector problem or to solve a linear equation system.

Example 3.4.1. Considering a bivariate vector

$$\mathbf{x} = \begin{bmatrix} X_1\\ X_2\end{bmatrix}, \quad \operatorname{Cov}(\mathbf{x}) = \boldsymbol{\Sigma} = \begin{bmatrix} 5 & 2\\ 2 & 2\end{bmatrix}$$

We want to find the principal components. What we need to solve is

$$\begin{gathered}(\boldsymbol{\Sigma} - \lambda_1\mathbf{I})\mathbf{a}_1 = \mathbf{0}\\ \left[\begin{bmatrix} 5 & 2\\ 2 & 2\end{bmatrix} - \lambda_1\begin{bmatrix} 1 & 0\\ 0 & 1\end{bmatrix}\right]\mathbf{a}_1 = \mathbf{0}\\ \begin{bmatrix} 5-\lambda_1 & 2\\ 2 & 2-\lambda_1\end{bmatrix}\begin{bmatrix} a_1\\ a_2\end{bmatrix} = \begin{bmatrix} 0\\ 0\end{bmatrix}\end{gathered}$$

where λ_1 is our unknown and we rewrote $\mathbf{a}_1$, the vector of coefficients we're looking for, as $\mathbf{a}_1 = \begin{bmatrix} a_1\\ a_2\end{bmatrix}$.
In order to have a nontrivial solution we need that determinant to be null

$$\begin{aligned}\begin{vmatrix} 5-\lambda_1 & 2\\ 2 & 2-\lambda_1\end{vmatrix} &= 0\\ (5-\lambda_1)(2-\lambda_1) - 2\cdot 2 &= 0\\ 10 - 5\lambda_1 - 2\lambda_1 + \lambda_1^2 - 4 &= 0\\ \lambda_1^2 - 7\lambda_1 + 6 &= 0\\ (\lambda_1 - 6)(\lambda_1 - 1) &= 0\end{aligned}$$

thus $\lambda_1 = 6, \lambda_2 = 1$ are the two eigenvalue of Σ, which are the variances of the two principal components: 6 will be the variance of the first PC and 1 the

variance of the second one.
To find the corresponding eigenvectors we comes back to our linear system:

$$\begin{bmatrix} 5-\lambda_1 & 2 \\ 2 & 2-\lambda_1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Now since $\lambda_1 = 6$ (consider first PC) we have

$$\begin{bmatrix} 1 & 2 \\ 2 & -4 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$
$$\begin{cases} -a_1 + 2a_2 = 0 \\ 2a_1 - 4a_2 = 0 \end{cases}$$

In order now to solve this system of equations (eg say by substitution) we run in first problem: the second equation is the first one multiplied by -2: so we have a single equation with 2 unknown.
But up to now we didn't used the unit norm constraint, which become useful/comes into play, so we add to the first equation:

$$\begin{cases} -a_1 + 2a_2 = 0 \\ a_1^2 + a_2^2 = 1 \qquad (\mathbf{a}_1^\top \mathbf{a}_1 = 1) \end{cases}$$

Now we use substitution taking a_1 in the first equation

$$\begin{cases} a_1 = 2a_2 \\ 4a_2^2 + a_2^2 = 1 \end{cases} \quad \begin{cases} \text{''}\,\text{''} \\ 5a_2^2 = 1 \end{cases} \quad \begin{cases} \text{''}\,\text{''} \\ a_2^2 = \frac{1}{5} \end{cases} \quad \begin{cases} \text{''}\,\text{''} \\ a_2^2 = \pm\sqrt{\frac{1}{5}} \end{cases}$$

I *decide* to take the positive root so

$$\begin{cases} a_1 = \frac{2}{\sqrt{5}} \\ a_2 = \frac{1}{\sqrt{5}} \end{cases} \implies \mathbf{a}_1 = \begin{bmatrix} \frac{2}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} \end{bmatrix}$$

This is my vector $\mathbf{a}_1$, the vector of coefficients of the first principal components. One could have either/also taken the negative root/solution obtaining

$$\begin{cases} a_1 = -\frac{2}{\sqrt{5}} \\ a_2 = -\frac{1}{\sqrt{5}} \end{cases}$$

These vectors are the same for our interest: the direction (pendenza) is the same. Thus principal component are uniquely defined up to sign changes (which can change from software to software. It depends on the software we use which solution is provided.
Let's calculate the second PC. Considering $\lambda_2 = 1$ we have

$$\begin{bmatrix} 5-1 & 2 \\ 2 & 2-1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$
$$\begin{cases} 4a_1 + 2a_2 = 0 \\ 2a_1 + a_2 = 0 \end{cases}$$

Again we take one of the two equations only (the second) since are linear combinations and add the unity norm constraint

$$\begin{cases} 2a_1 + a_2 = 0 \\ a_1^2 + a_2^2 = 1 \end{cases} \quad \begin{cases} a_2 = -2a_1 \\ a_1^2 + 4a_1^2 = 1 \end{cases} \quad \begin{cases} "" \\ 5a_1^2 = 1 \end{cases} \quad \begin{cases} "" \\ a_1^2 = \pm\frac{1}{\sqrt{5}} \end{cases}$$

Taking the positive root we end with

$$\begin{cases} a_1 = \frac{1}{\sqrt{5}} \\ a_2 = -\frac{2}{\sqrt{5}} \end{cases} \implies \mathbf{a}_2 = \begin{bmatrix} \frac{1}{\sqrt{5}} \\ -\frac{2}{\sqrt{5}} \end{bmatrix}$$

Note that while the vector of first component have all positive (or negative) elements if we want an orthogonal second component we need something that null the product of the two vectors so it will be of mixed signs (some elements will be positive and some negative).

Important remark 16. Let's appreciate two relevant aspects in the previous example:

1. the first eigenvector 6 is larger than any entries on the diagonal of original covariance matrix $\mathbf{\Sigma}$ (5 and 2). That is: the variance of the first principal component (6) is higher than any variance of the original variable.
   In general the variance of the first PC will *never* be smaller than the largest observed variance: it can be that the variance is equal but will be never be below;

2. looking at the trace of $\mathbf{\Sigma}$ it's 5+2; the sum of the eigenvalues is still 6+1=7. This always holds, so:

   $$\sum_{i=1}^{p} \mathrm{Var}[X_i] = \sum_{k=1}^{p} \lambda_k$$

   Remembering that the PCs are uncorrelated, we can write the variance covariance matrix of the PC as a matrix $\mathbf{\Lambda}$:

   $$\mathbf{\Lambda} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$

   the off diagonal elements is always $= 0$ (being PCs uncorrelated). Thus we can rewrite

   $$\mathrm{Tr}\,\mathbf{\Sigma} = \mathrm{Tr}\,\mathbf{\Lambda}$$

   So if one sum the eigenvalue variance of principal components it get the same variability of the original variable (trace of covariance matrix).
   Through PC we obtain a different way to split variability, we are not changing the total variability.

3. in general if first PC is a strict linear combinations (all entries with same sign), then the following (second and 3rd and so on) need/will be a contrast (different sign) in order orthogonality to be satisfied (vector product will be 0).

3.4.1 Matrix A and principal components

Remark 20. We can collect all eigenvector in a matrix called $\mathbf{A}$ (fof p variables $\mathbf{A}$ is a $p \times p$ matrix), whose columns are the eigenvector of $\mathbf{\Sigma}$ ordered according to decreasing values of the corresponding eigenvalues $\mathbf{\Sigma}$

$$\underset{p\times p}{A} = \begin{bmatrix}\mathbf{a}_1 & \mathbf{a}_2 & \dots & \mathbf{a}_p\end{bmatrix}$$

Example 3.4.2. In the example above

$$\mathbf{A} = \begin{bmatrix}\mathbf{a}_1 & \mathbf{a}_2\end{bmatrix} = \begin{bmatrix}\frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} & -\frac{2}{\sqrt{5}}\end{bmatrix}$$

Important remark 17 (Properties of $\mathbf{A}$). Matrix $\mathbf{A}$ has orthogonal columns and so

$$\mathbf{A}^\top \mathbf{A} = \mathbf{I}$$

this because eigenvector have unit norm (so in the diagonal $\mathbf{a}_i^\top \mathbf{a}_i = 1$) and are orthogonal (so out of main diagonal $\mathbf{a}_i^\top \mathbf{a}_j = 0$).

Definition 3.4.1 (Vector of principal components). Once collected $\mathbf{A}$ we can write in matrix form the vector of principal components $\mathbf{y}$ as product of $\mathbf{A}$ and the vector of observed variables:

$$\underset{p\times 1}{\mathbf{y}} = \underset{p\times p}{\mathbf{A}^\top}\,\underset{p\times 1}{\mathbf{x}}$$

We previously seen that:

1. the variance of multiple linear combinations $\mathbf{Ax}$ is

$$\text{Var}\left[\mathbf{y}\right] = \mathbf{A}^\top \text{Var}\left[\mathbf{x}\right] \mathbf{A} = \underbrace{\mathbf{A}^\top}_{p\times p}\underbrace{\mathbf{\Sigma}}_{p\times p}\underbrace{\mathbf{A}}_{p\times p}$$

2. covariance of principal component is 0; $\mathbf{\Lambda}$ has eigenvalue in decreasing order and out of diagonal we have 0

$$\underset{p\times p}{\mathbf{\Lambda}} = \begin{bmatrix}\lambda_1 & \dots & 0 & \dots & 0 \\ \dots & & & & \\ 0 & \dots & \lambda_i & \dots & 0 \\ \dots & & & & \\ 0 & \dots & 0 & \dots & \lambda_p\end{bmatrix}$$

3. thus holds the following equivalence

$$\text{Var}\left[\mathbf{y}\right] = \mathbf{A}^\top \mathbf{\Sigma} \mathbf{A} = \mathbf{\Lambda}$$

so $\mathbf{\Sigma}$ and $\mathbf{\Lambda}$ *are similar*, considered that $\mathbf{A}^\top = \mathbf{A}^{-1}$ being $\mathbf{A}$ orthogonal.

Important remark 18 (Similar matrices (reminder)). Two matrices $\mathbf{X}$ and $\mathbf{Y}$ are similar if there exists a non-singular matrix $\mathbf{Z}$ such that $\mathbf{Z}^{-1}\mathbf{YZ} = \mathbf{X}$.

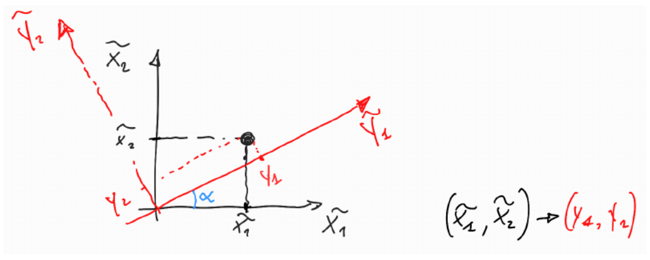


Figura 3.1: Rotation

Important remark 19. Similar matrices share many properties: among them they have the same trace. So $\operatorname{Tr} \boldsymbol{\Sigma} = \operatorname{Tr} \boldsymbol{\Lambda}$ and this is the proof that variances of observed variances coincides with sum of variances of principal components. Thus PC transform data but doesn't change total variability.

Important remark 20. Actually what PCA does is to *apply the spectral decomposition to covariance matrix*: this is interesting from the statistical point of view in order to have uncorrelated new variables and same total variances (represented by eigenvectors).

3.5 Interpretation

What does we do when we perform PC? 3.1 Let's assume variables are mean centered for simplicity and that we want to rotate the reference system.
The original point (x_1, x_2) will be transported in the new reference system and will be transformed to (y_1, y_2). Clearly the coordinates are linked and it turns out that the coordinates on the new sistem depend on the angle between red and black line (α): if one change it, change the coordinates of the points.
Relationship between coordinates of two reference systems turns out to be:

$$\begin{cases} y_1 = x_1 \cos\alpha + x_2 \sin\alpha \\ y_2 = -x_1 \sin\alpha + x_2 \cos\alpha \end{cases}$$

We can collect the coefficient of the rotation/linear combination in

$$\mathbf{a}_1 = \begin{bmatrix} \cos\alpha \\ \sin\alpha \end{bmatrix}, \quad \mathbf{a}_2 = \begin{bmatrix} -\sin\alpha \\ \cos\alpha \end{bmatrix}$$

but $\cos^2\alpha + \sin^2\alpha = 1$ so both $\mathbf{a}_1, \mathbf{a}_2$ are unit norm vector. Moreover

$$\mathbf{a}_1^\top \mathbf{a}_2 = -\cos\alpha \sin\alpha + \sin\alpha \cos\alpha = 0$$

Important remark 21. So these vectors (depending on *alpha*) are orthogonal and with unit norm, as PCA'S are. This means that:

- we can think PCA as an **orthogonal rotation of the reference system**.
- we have an infinity of possible orthogonal rotations (rotations are infinite, as *alpha*'s are): the one corresponding to PC is such that the **spread on the point of the first component is the maximum**.

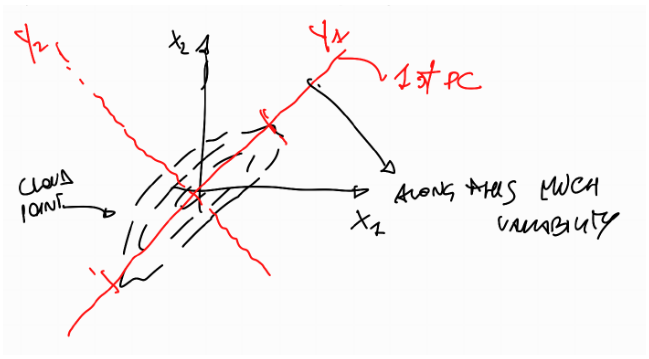


Figura 3.2: Pca popularity

- performing PC is just changin the reference system: actually we choose the optimal α with PC; trace remains the same because we're just rotating the system not changing data.

Important remark 22 (PCA vs FA). PCA is just a data transformation (orthogonal rotation) procedure and *always is feasible*: one can always move from X reference system to Y's one.
OTOH factor analysis has many things in common but *it is a model* and not necessarily *exists or appropriate*

Important remark 23 (Reason popularity of PC). Reason of the popularity is because it allows us to collapse multidimensionality; eg in a situation like this (mean centered varaible for simplicity).
In figure 3.2 Along the first pc the variability is higher, along the second a bit less: the core of data is along Y_1, remaining part could be noise.

Important remark 24. In general however we need *formal criteria* to choose the *number of components* which are enough to summarize the data. There are different answers to this. Before considering this let's see the sad side of the story for PC

3.6 Dependance on units of measure

Consider the following situations with two covariance matrix equal in all but in the units

$$\mathbf{\Sigma}_1 = \begin{bmatrix} 90 & 50 \\ 50 & 90 \end{bmatrix}, \quad \mathbf{\Sigma}_2 = \begin{bmatrix} 9000 & 500 \\ 500 & 90 \end{bmatrix}$$

This is due to the fact that *data are the same* but in the first case X_1 is measured in cm, in the second case it is expressed in mm. Does the change in the measurement unit affect PCA results?
If we do spectral decomposition the following is obtained;

- for $\mathbf{\Sigma}_1$

$$y_1 = 0.707x_1 + 0.707x_2$$

  and $\lambda_1 = 140$. As we can see:

  - the variables are equally weighted/important (coefficients 0.707) equally in the first component;
  - trace of covariance matrix is 180, while variance explained by first PC is 140. Considering the first PC only, we take into account 78% of total variability.

- for Σ_2

$$y_1 = 0.998x_1 + 0.055x_2$$

  with $\lambda_1 = 9027.97$ and percentage explained is $\lambda_1/\operatorname{Tr}\Sigma_2 = 99.32$ %. So in this case:

  - coefficients are very different: the combination is completely dominated by x_1, while x_2 has a small coeff
  - the explained variance increase just because of the unit measure and the increased importance of x_1 in the PC solution

Important remark 25. This example tells us that *PCA is not scale equivariant*: it depends on units of measurement. The solutions we obtain can be completely different.
Often we don't want this to happen (that is our result to be dependent of the unit of measure).
So if we don't want results to be affected by units of measure standard practice is to **standardize before** (and considering the correlation matrix instead of the covariance one, we have seen that the covariance matrix of the standardized variables is the correlation matrix) and then to obtain eigenvalues and eigenvectors from the correlation matrix $\boldsymbol{\rho}$ (instead of the covariance).

3.6.1 Relationship between PCA on covariance and correlation matrixes

Remark 21. Is there a relationship between eigenvalues/vectors of Sigma and Corr? If that is so we could move from one solutions to the other?

We know that $\boldsymbol{\rho}$ (at the population level)

$$\boldsymbol{\rho} = \boldsymbol{\Delta}^{-1/2}\boldsymbol{\Sigma}\boldsymbol{\Delta}^{-1/2} \tag{3.3}$$

where $\boldsymbol{\Sigma}$ is analog of sample couterpart $\mathbf{S}$ and $\boldsymbol{\Delta}$ is analog of $\mathbf{D}$, that is

$$\boldsymbol{\Delta} = \begin{bmatrix} \sigma_1^2 & \dots & 0 & \dots & 0 \\ \dots & & & & \\ 0 & \dots & \sigma_i^2 & \dots & 0 \\ \dots & & & & \\ 0 & \dots & 0 & \dots & \sigma_p^2 \end{bmatrix}$$

from 3.3 this it's easy to obtain a new way to write the covariance matrix which show the *link between covariance and correlation matrix*

$$\boldsymbol{\rho} = \boldsymbol{\Delta}^{-1/2}\boldsymbol{\Sigma}\boldsymbol{\Delta}^{-1/2} \implies \boldsymbol{\Sigma} = \boldsymbol{\Delta}^{1/2}\boldsymbol{\rho}\boldsymbol{\Delta}^{1/2}$$

Now if $\mathbf{a}$ is an eigenvector of $\boldsymbol{\rho}$ and λ is the corresponding eigenvalue, we have for what seen so far (relationship be eigenval/vecs)

$$\boldsymbol{\rho}\mathbf{a} = \lambda\mathbf{a}$$

If $\mathbf{b}$ is an eigevector of $\boldsymbol{\Sigma}x$ and δ is the corresponding eigenvalue, we have as well:

$$\boldsymbol{\Sigma}\mathbf{b} = \delta\mathbf{b}$$

So

$$\begin{aligned}&\boldsymbol{\Sigma}\mathbf{b} = \delta\mathbf{b}\\&\boldsymbol{\Delta}^{1/2}\boldsymbol{\rho}\boldsymbol{\Delta}^{1/2}\mathbf{b} = \delta\mathbf{b}\end{aligned}$$

if we premultiply both sides to $\boldsymbol{\Delta}^{-1/2}$ on the left hand side we obtain

$$\boldsymbol{\rho}\boldsymbol{\Delta}^{1/2}\mathbf{b} = \delta\boldsymbol{\Delta}^{-1/2}\mathbf{b}$$

now we decide/rename that $\mathbf{c} = \boldsymbol{\Delta}^{1/2}\mathbf{b}$ so

$$\boldsymbol{\rho}\mathbf{c} = \delta\boldsymbol{\Delta}^{-1}\mathbf{c}$$

Is this an eigenvalue-eigenvector relationship for $\boldsymbol{\rho}$? $\mathbf{c}$ is eigengevector of $\boldsymbol{\rho}$ only if $\boldsymbol{\Delta}^{-1}\mathbf{c} = \mathbf{c}$, but $\boldsymbol{\Delta}^{-1}\mathbf{c} \neq \mathbf{c}$ because $\boldsymbol{\Delta} \neq \mathbf{I}$ (it's the matrix of variances of variables). So $\boldsymbol{\rho}\mathbf{c} = \delta\boldsymbol{\Delta}^{-1}\mathbf{c}$ is not an eigenvalue-eigenvector relationship.
This tells us that the eigenvalues and eigenvectors of $\boldsymbol{\Sigma}$ are different from the eigenvalues/vectors of $\boldsymbol{\rho}$ and there is no way to move from one solutions to the other.

Important remark 26. So NO, there's no relationship between eigenvalues/vectors of Σ and $\boldsymbol{\rho}$. When performing PCA we need to decide *before* to standardize or not: if we have

1. different units of measuremente or
2. very different variances

then standardize variables is better.
Otherwise if differences in variances are important and we don't want to homogeneize it, then use the covariance unstandardized matrix.

Example 3.6.1. Consider

$$\boldsymbol{\rho} = \begin{bmatrix}1 & \rho\\ \rho & 1\end{bmatrix}$$

derive principal components, what changes when ρ is positive or negative?

3.7 Number of components to choose

Now we look into criteria to decide how many components we need/take to at the sample level. We estimate $\boldsymbol{\Sigma}$ or $\boldsymbol{\rho}$ (in the population) with ML estimators:

- for $\boldsymbol{\Sigma}$ we use $\mathbf{S}$ (the ML estimates for $\boldsymbol{\Sigma}$, dividing codeviances by n). If we prefer we could use the unbiased estimate for $\boldsymbol{\Sigma}$ (dividing codeviances by $n-1$ instead of n); the variance of the principal components will be rescaled accordingly and the eigenvectors will not change;
- for $\boldsymbol{\rho}$ we use $\mathbf{R}$ where the same happens.

Important remark 27. How can we decide how many PCs we should keep in order to reduce dimensionality and at the same time preserve as much info as possible? We have a tradeoff: we want to reduce dimensionality but don't want to loose to much information.
We have different rule of thumb (not formal criteria, suggestion based on empirical evidence) to select the number n of principale components:

1. percentage of explained/retained variance
2. threshold on eigenvalue
3. screeplot

For each criteria we have two "variants" which depend on if we work with $\mathbf{S}$ or $\mathbf{R}$.
Important remark 28 (Why rule of thumbs). The reason why there's no formal criteria is because so far we made no assumption on distribution of variables: PC are data transformation and such can be always obtained (it's just an algebraic procedure done on covariance matrix or correlation matrix). In principle we don't need info on population: as it's very general the only way we have to make decision is to use empirical rules (in essence it's a descriptive method).

3.7.1 Percentage of explained variance

Common to both strategies (starting from $\mathbf{S}$ or $\mathbf{R}$) is cumulative percentage of explained/retained variance. For what concerns:

- $\mathbf{S}$: we know that the
$$\operatorname{Tr}\mathbf{S} = \operatorname{Tr}\mathbf{L} = \sum_{i=1}^{p} s_i^2 = \sum_{k=1}^{p} l_k$$
where $\mathbf{L}$ is the matrix with the eigenvalues (the sample analog of $\boldsymbol{\Lambda}$), while s_i^2 are the observed variances.
The proportion of total variance explained by first PC is
$$\frac{l_1}{\operatorname{Tr}\mathbf{L}} \cdot 100$$
The proportion explained by first twos is
$$\frac{l_1 + l_2}{\operatorname{Tr}\mathbf{L}} \cdot 100$$
The percentage explained up to m components is
$$\frac{\sum_{k=1}^{m} l_k}{\operatorname{Tr}\mathbf{L}} \cdot 100$$
The criteria is to stop cumulating at the value m that make the above explained $\geq 80\%$

- **R**: similarly we have that
$$\operatorname{Tr}\mathbf{R} = \operatorname{Tr}\mathbf{L} = \sum_{i=1}^{p} 1 = \sum_{k=1}^{p} l_k = p$$
where we substituted the variance s_i^2 with 1, that is the correlation of each variable with itself. So with standardized data the total variance ($\operatorname{Tr}\mathbf{R}$) is just the number of variables p.
The reasoning is the same but percentage of explained by first component is now
$$\frac{l_1}{p} \cdot 100$$
And again the final criteria is:
$$\frac{\sum_{k=1}^{m} l_k}{p} \cdot 100 \geq 80\%$$

Remark 22. R has two procedures (one based on spectral decomposition one based on Singular value decomposition) but eigenvector are the same.

3.7.2 Threshold on eigenvalues (Kaiser's rule)

For the second rule, known as Kaiser's rule, we start seeing this applied correlation matrix (it was invented when working with standardized variable). For:

- **R**: we keep as many principal components as are the eigenvalues ≥ 1: in order to keep the principal components that do better than original variabiles (which have variance 1 being standardized). So 1 act as a treshold to select the number of PCs;

- **S**: lets consider what 1 is for the correlation matrix above and find an equivalent for **S**. 1 is also the *average eigenvalue/variance* (sum of eigenvalues is p divided by number of elements p). Therefore we can translate the Kaiser's rule in the non standardized world by keeping as many PCs as are the eigenvalues of **S** which are $\geq$ than the mean variance/eigenvalue:
$$\bar{l} = \frac{\sum_{k=1}^{p} l_k}{p}$$

Important remark 29 (Joliffe's variant). In some books a slightly modified version of the rule above (due to Joliffe) are found:

- for **R**: considering that I'm working in a sample if I reject eigenvalues below 1/mean it may be that I'm refusing something that in the population is above 1/mean and the sample was "particular".
In other words, variability slightly lower than 1 can be kept/retained if in the population are actually 1 or more.
After some simulation Joliffe ended with choosing to lower the sample treshold to 0.7 (instead of 1);

- in the case of unstandardized data we use $0.7 \cdot \bar{l}$

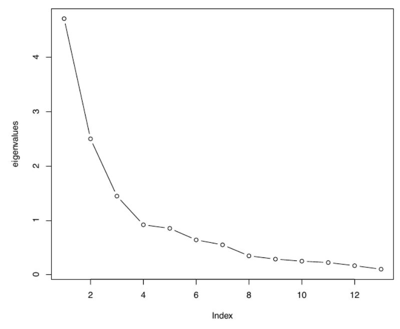


Figura 3.3: Screeplot

3.7.3 Screeplot

It's a graphical rule common to both matrix **S** and **R**. We plot the eigenvalues in order from the highest to the lower to describe the fall/slope (fig 3.3).
At some point in the graph there will be an *elbow*: when the lines stop decreasing a lot and becomes almost flat, all the PC passed that point capture the same amount of variability (so we can either take one of them or we throw them all away).
The rule is: keep as many PC as are the eigenvalues *preceding* the elbow point (that is the point from which the screeplot becomes flat so in the example above we should have taken 3/4 PC)

3.8 PC interpretation

How do we interpret principal components? Assume we have two variables (height and weight) and that the variables are mean centered (just to ease graph without losing generality). There are **two strategies** to do it:

- one way we do by looking at the *extremes* (look at coefficients/element of eigenvector). We study sign and the value of the elements of the eigenvectors and try to figure out what happens at the extremes.
  Important: remember that eigenvector has unit norm: if norm is unit we can measure the importance of each variable for a component and look how variables balance in the vector (this is the prof favorite method).
  Most of the case first PC have the same sign on all elements of the eigenvector (not always, but often is like that), while the other are contrasts.

- otherwise we look at the *correlation* between each principal component and the observed variables

3.8.1 Extremes interpretation

Strategy is to look at extremes and name the pc according to these extremes; the method is called *reification of PC* (give meaning to math construct from an empirical point of view).
Looking at fig 3.4 if we project the point:

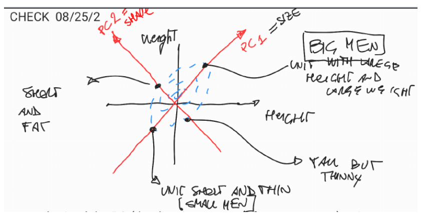


Figura 3.4: PCA interpretation using extremes

- into the first direction we're able to order individuals on the "size" variable: looking at the first component at one end we have mes with high height/weight (BIG men) at the other low height/weight (SMALL men);
- along the second orthogonal direction we have that are characterizing individual according to the "shape": on one hand we have short and fat men, on the other tall but thin

Example 3.8.1. Before looking at a second criteria of interpreting the PCs we see a popular example with 6 variables on chicken (*galline bianche sperone*, white leghorn chicken) which are:

- length cranium (head)
- width cranium (head)
- length humerus (wing)
- length ulna (wing)
- length femur (legs)
- length of tibia (legs)

with 6 variables we have up to 6 PC: the example is famous because to all 6 components we can give a meaning! (usually is not that so).
Data available is on correlation matrix (we have a 6x6 matrix only): with R's `eigen` we calculates eigenvalues and vectors eigenvalues:

- the first PC accounts for 76%, while the first two we have more than 80% (so 2 are enough according to proportion of explained variance).
- applying Kaiser's rule we would conclude that 1 PC is enough; to lower the bound according to Joliffe we take two PC (second has eigenvector 0.71)

Our focus is now interpreting: each column corresponds to an eigenvector, plotted in the order of the corresponding eigenvalues so vectors matrix is our **A**

1. the first eigenvector is composed of all negative coefficients (could be positive either): looking at elements of the vector (their absolute value) they are more or less the same (between 0.3 and 0.4): to interpret (assume is positive to ease) what a chicken with an high value on the first principal components looks like?

$$Y_1 \approxeq 0.3(x_1 + x_2) + 0.4(x_3 + x_4 + x_5 + x_3)$$

a chicken with large first PC1 will be big while small values will correspond to small chicken; so PC1 describes the *size* of the chicken;

2. the second is a contrast (not all are the same) otherwise they are not orthogonal: we have positive values with two variables describing the head and negative values for wings and legs. I need a large value of positive. High score on the second are for chicken with large head and small body, low scores small head and big body.

$$Y_2 \approx 0.6(x_1 + x_2) - 0.2(x_3 + ... + x_6)$$

so PC2 can be seen as a "shape" (large/small head vs body).
These are the main two components; most variability of the chicken are related to size and shape

3. if we go on and consider the third PC: values with body characteristics are really near to 0 so I can ignore this, only the head variables is important

$$y_3 \approx 0.77x_1 - 0.63x_2$$

I have again a contrast (because of the sign): on one side chicken with long head and not large, on the other side short and large head. So this third PC describes "head shapes"

4. the fourth PC neglect/ignore the head data. We focus on legs and wings

$$y_4 = -0.5(x_3 + x_4) + 0.5(x_5 + x_6)$$

large positive values correspond to chicken with big legs and small wings, on the other side large wings and small legs (another measure of shape of the body)

5. and so on ...

Example 3.8.2. Recent paper (global spectrum of plant form and function (Sandra Diaz: most famous living ecologist Argentinian) published in nature main characteristics of plants all around the world.
They were able to define 2 PC starting from 6 variables of plants from all over the world.
Variables considered on 46000 plants are length, stem density (how much production), leaf size/area, leafs mass (how heavy), leaf nitrogen content and diaspora mass.
The combinations of 6 features found to be in a two dimensional space which can be plotted.
Two principal components were enough and plotted all the plants; heatmap displays density and two cluster emerged. The first goes from small plants to very big plants (moving from left to right, while the second pc (from below to above) describes the size of the leaves (from to very broad to very thin).
Finally it is shown a *biplot*: two variables (original variables and pc) plotted in the same plot.

3.8.2 Correlation between PC and variables

What is the correlation between each principal component and the observed variables? We're interested in $cov(y_1, \mathbf{x})$ with y_1 is a scalar random variable (1×1), $\mathbf{x}$ is a vector of observed variable ($px1$ vector).
If we assume to work with *mean centered* observation $\mathbf{x}$, the covariance is

$$\text{Cov}\left(y_1, \mathbf{x}\right) = \mathbb{E}\left[y_1 \mathbf{x}\right] \overset{(1)}{=} \mathbb{E}\left[\mathbf{a}_1^\top \mathbf{x}\mathbf{x}^\top\right] \overset{(2)}{=} \mathbf{a}_1^\top \,\mathbb{E}\left[\mathbf{x}\mathbf{x}^\top\right] = \mathbf{a}_1^\top \boldsymbol{\Sigma}$$

where in

- (1) we just replaced the first principal component.
- (2) $\mathbf{a}_1$ is a constant vector that can be taken out of expectation

Thus the covariance between y_1 and $\mathbf{x}$ is $\mathbf{a}_1^\top \boldsymbol{\Sigma}$. But also we have that

$$\mathbf{a}_1^\top \boldsymbol{\Sigma} = \lambda_1 \mathbf{a}_1^\top$$

Now the correlation

$$\text{Corr}\left(y_1, \mathbf{x}\right) = \frac{1}{sd(y_1)} \cdot \text{Cov}\left(y_1, \mathbf{x}\right) \cdot \boldsymbol{\Delta}^{-1/2}$$

at the last passage we needed to derive by the standard deviation of $\mathbf{x}$ (usual diagonal matrix Δ). Now we have a problem: we need to define the standard deviation of first PC: which is the $sd(y_i)$? it's the $\sqrt{\text{Var}\left[y_i\right]} = \sqrt{\lambda_1}$

$$\begin{aligned}\text{Corr}\left(y_1, \mathbf{x}\right) &= \frac{1}{\sqrt{\lambda_1}} \lambda_1 \mathbf{a}_1^\top \boldsymbol{\Delta}^{-1/2} \\ &= \sqrt{\lambda_1} \mathbf{a}_1^\top \boldsymbol{\Delta}^{-1/2}\end{aligned}$$

in the sample the formula to adopt is

$$\text{Corr}\left(y_1, \mathbf{x}\right) = \sqrt{l_1} \mathbf{a}_1^\top \mathbf{D}^{-1/2}$$

TODO: check 09/26, risentire

corr is a function of vector $\mathbf{a}_1^\top$ but while elements are constrained to be unit norm, here we just work with pairwise correlation. with these way we loose the multivariate feelings

Important remark 30 (PCA and factor analysis). Speaking about factor analysis we will see that there are connection with PC: PCA can be obtained using the same code used for fittining a factor analytics models, by putting some constraints. This is useful from programming pov because with one procedure we have two tools at our disposal.
However this caused a lot of confusion, people think that two methods are equivalent (thinking one of them is special case of other) so people used methods from factor analysis on PC (eg rotating principal components to improve interpretability, a thing is usually done in factor analyis): this thing drives prof crazy.
PC is an axis rotation done in order to maximize the variability explained. We've seen that PC solution is unique (but sign). This means that *if we rotate it to improve interpetability we have no more PC* (we obtain something that is easier to interpret but no longer the obtained first PCs optimize the explained variability).

3.9 Principal component scores

Scores are nothing but values of each components y. Dealing with sample data (and multiple components) we have $\mathbf{Y}$ which is $n \times p$ matrix which contains the coordinates of the n units in the space spanned by the p principal components. In this matrix we have for each unit the element of $\mathbb{R}^p$ from the components. It is obtained as

$$\underset{n\times p}{\mathbf{Y}} = \underset{n\times p}{\mathbf{X}}\underset{p\times p}{\mathbf{A}}$$

where $\mathbf{X}$ is original data matrix and $\mathbf{A}$ is the matrix of the eigevectors.
If we don't want to keep all the PCs but only m we'll have

$$\underset{n\times m}{\mathbf{Y}_m} = \underset{n\times p}{\mathbf{X}}\underset{p\times m}{\mathbf{A}_m}$$

where $\mathbf{A}_m$ is the matrix containing the first m eigenvectors.

3.10 Importance of last PCs

Now, focusing on the last PC, is it useful? the last PC have a meaning and there are at least two situations in which last PC is important

3.10.1 Goodness of first PCs

TODO: CHECK 09 26(2

Assume we performed PC in this room (x,y,z of object in space): two points/components are enough to project students head/position on the floor but if we project the lamp too it will be near the students over it is (despite being distant from them in 3d space).
How can we measure the *quality of representation*: if there's a unit that is very distant (lamp) from the other how can we say this? It turns out that the *coordinates along the last PC are a measure the quality of the first PCs.*
I can measure the distance of each units from the projection using only the first m PCs: this below is a measure of the quality of the m dimensional representation (using only the first m principal components) of unit j.

$$y_{j,m+1}^2 + y_{j,m+2}^2 + \ldots + y_{j,p}^2$$

If the measure above is much larger than its average, with respect to all the units, then this means that unit j is badly represented by m PCs alone.
Idea is: last PCs cannot be thrown away since they provides us goodness of the first PCs.

3.10.2 Multicollinearity

TODO: CHECK 09 26

Another possible use of last PC is in multicollinearity diagnosis (for linear regression), other than methods such as VIF.
Multicollinearity means in regression that in the $\mathbf{X}$ we have one column is almost a combination of other vectors. If this is so, we can use PC to spot it: If there are eigenvalue close to 0 there's multicollinearity in data.

3.11 PCA and SVD

SVD is a matrix decomposition, way to decompose matrix $\mathbf{X}$, that tells us that given an $n \times p$ matrix $\mathbf{X}$, we can decompose it it in the product of three matrices

$$\underset{n\times p}{\mathbf{X}} = \underset{n\times p}{\mathbf{U}}\underset{p\times p}{\mathbf{P}}\underset{p\times p}{\mathbf{V}^\top}$$

where:

- $\mathbf{X}$ is the data matrix;
- $\mathbf{U}$ is the matrix of the left singular vectors (that is the eigenvectors of $\mathbf{X}\mathbf{X}^\top$ corresponding to non 0 eigenvalues). Note that $\mathbf{X}\mathbf{X}^\top$ is not we used so far ($\mathbf{X}^\top\mathbf{X}$) $\mathbf{X}\mathbf{X}^\top$ is $n \times n$ and has ;

TODO: CHECK

- $\mathbf{P}$ is a square diagonal matrix, whose diagonal entries are the *singular values* of $\mathbf{X}$, which are the square root of the non zero eigenvalues of $\mathbf{X}\mathbf{X}^\top$ (or $\mathbf{X}^\top\mathbf{X}$, as the two matrices have the same eigenvalues)
- $\mathbf{V}$ is the *matrix of right singular vectors* (i.e. the eigenvectors of $\mathbf{X}^\top\mathbf{X}$)

Now let's assume we work on mean centered data and consider $\tilde{\mathbf{X}}$; the codeviance matrix (numerator of covariance matrix) can be written as product of n times the covariance matrix

$$\tilde{\mathbf{X}}^\top\tilde{\mathbf{X}} = n\mathbf{S}$$

From matrix algebra it turns out that:

- $\tilde{\mathbf{X}}^\top\tilde{\mathbf{X}}$ and $\mathbf{S}$ have the *same eigenvectors* (what changes is only eigenvalues). From PCA, we know that eigenvectors of $\mathbf{S}$ are the elements of matrix $\mathbf{A}$ (solution to the PC problems): so $\mathbf{A}$ will be the matrix of the eigenvectors of both $\tilde{\mathbf{X}}^\top\tilde{\mathbf{X}}$ and $\mathbf{S}$.
- the eigenvalues of $\mathbf{S}$ will be the eigenvalues of $\tilde{\mathbf{X}}^\top\tilde{\mathbf{X}}$ divided by n

Thus if we consider the singular value decomposition of $\tilde{\mathbf{X}}$ we have

$$\tilde{\mathbf{X}} = \mathbf{U}\mathbf{P}\mathbf{A}^\top$$

going back to the PC scores $\mathbf{Y}$, we can replace $\tilde{\mathbf{X}}$ with its SVD:

$$\mathbf{Y} = \tilde{\mathbf{X}}^\top\mathbf{A} = \mathbf{U}\mathbf{P}\mathbf{A}^\top\mathbf{A} \overset{(1)}{=} \mathbf{U}\mathbf{P}$$

where in (1) since $\mathbf{A}$ is orthogonal so $\mathbf{A}^\top\mathbf{A} = \mathbf{I}$.

Important remark 31. So using SVD we obtained all the main elements of PC analysis:

- $\mathbf{A}$ (of PCs) is $\mathbf{V}$ (in the Svd decomposition)
- $\mathbf{U}\mathbf{P}$ is the matrix with the PC scores $\mathbf{Y}$ (where the diagonal matrix $\mathbf{P}$ is $\mathbf{P} = n^{1/2}\mathbf{L}^{1/2}$)

So we can obtain PC either by spectral decomposition or by SVD of centered data matrix.

Important remark 32. Moreover if we consider only m principal components then we will have that:

$$\tilde{\mathbf{X}} \approxeq \mathbf{U}_m \mathbf{P}_m \mathbf{V}_m^\top$$

there's a theorem due to Eckart and young that states that the equation above is the best rank m approximation of $\tilde{\mathbf{X}}$: no other rank m approximation are better than this.[4]

TODO: CHECK 09/26

3.12 Lab

We do PCA both manually and results are different from functions.
Generally, PCA aims to find the linear combinations of the observed variables which explain as much of the data variability as possible. Besides, this method is implemented to perform dimension reduction, i.e. to produce a smaller set of uncorrelated variables from the larger set of correlated ones.

3.12.1 Example 1: Job performance

Data contain observations on fifty police officers that were rated by their supervisors in 6 categories as part of standard police departmental administrative procedure:

- `commun`: Communication Skills
- `probl_solv`: Problem Solving
- `logical`: Logical Ability
- `learn`: Learning Ability
- `physical`: Physical Ability
- `appearance`: Appearance

```
job <- read.table("data/job_perf.txt", header = TRUE)
head(job) # 6 var

##   commun probl_solv logical learn physical appearance
## 1     12         52      20    44       48         16
## 2     12         57      25    45       50         16
## 3     12         54      21    45       50         16
## 4     13         52      21    46       51         17
## 5     14         54      24    46       51         17
## 6     14         48      20    47       51         18

summary(job)
```

[4]YouTube: SVD song it had to be U - the SVD song statistical song youtube michael greenacree

```
##      commun         probl_solv       logical          learn      
##  Min.   :12.00   Min.   :48.00   Min.   :20.00   Min.   :44.00  
##  1st Qu.:16.00   1st Qu.:52.25   1st Qu.:22.00   1st Qu.:48.00  
##  Median :18.00   Median :54.00   Median :24.00   Median :50.00  
##  Mean   :17.68   Mean   :54.16   Mean   :24.02   Mean   :50.28  
##  3rd Qu.:19.75   3rd Qu.:56.00   3rd Qu.:26.00   3rd Qu.:52.00  
##  Max.   :24.00   Max.   :59.00   Max.   :31.00   Max.   :56.00  
##     physical       appearance   
##  Min.   :48.00   Min.   :16.00  
##  1st Qu.:52.25   1st Qu.:19.00  
##  Median :54.00   Median :21.00  
##  Mean   :54.16   Mean   :21.06  
##  3rd Qu.:56.00   3rd Qu.:23.00  
##  Max.   :59.00   Max.   :28.00

## to perform PCA manually we use matrix computation
X <- as.matrix(job) # first transform to matrix
n <- nrow(job)      # we need number of obs in our dataset

# we should check that variables are correlated prior to performing
cor(X)

##               commun probl_solv   logical     learn  physical appearance
## commun     1.0000000  0.1313258 0.2252998 0.9821863 0.9767974  0.9692466
## probl_solv 0.1313258  1.0000000 0.3637625 0.1425815 0.1640910  0.1287805
## logical    0.2252998  0.3637625 1.0000000 0.2307109 0.2582155  0.2164945
## learn      0.9821863  0.1425815 0.2307109 1.0000000 0.9814717  0.9718918
## physical   0.9767974  0.1640910 0.2582155 0.9814717 1.0000000  0.9690222
## appearance 0.9692466  0.1287805 0.2164945 0.9718918 0.9690222  1.0000000
```

Is PCA justified? It is possible to reduce data dimensionality without losing too much information only if the original variables are highly correlated. In fact, when the correlation between variables is weak, a larger number of components is needed in order to capture enough variability.

Is PCA justified? Here yes, Since the correlation values look quite large (eg `learning` and `phisical` and `appearance` with `commun`), in this context PCA seems to be useful in order to reduce dimensionality.

Should the PCA be carried out with the covariance or the correlation matrix? To choose between the covariance and the correlation matrix is like to choose whether to work with standardized variables or not. Indeed, the correlation matrix of X coincides with the covariance matrix if the variables are standardized.

The use of correlation matrices (that is standardized variables) is recommended when the magnitudes of the variables are very different. Indeed, the latter implies different variance magnitudes, which would imply that the first few principal components are dominated by the variables with bigger magnitudes. Standardization gives to all the variables the same importance in determining the components. Since in this example the variances are quite similar, it is possible to use the covariance matrix to carry out PCA.

```
## we need to chose if work with standardized data or not. To choose it we can
## look at variances of variables. Either using diag(S) or using apply/lapply

apply(X, 2, var)

##     commun probl_solv    logical      learn   physical appearance
##   7.528163   5.810612   6.183265   8.042449   5.810612   8.955510

# var have the similar variances it's not needed to work with standardized
# data. For this dataset we can work with covariance matrix
## to compute PCA do spectral decomposition (using eigen function)
```

3.12.1.1 PCA using matrix functions

In order to perform PCA we need to do spectral value decomposition of covariance/correlation matrix: here we chose to do it on covariance matrix. So the decomposition become

$$\mathbf{A}^\top \mathbf{S} \mathbf{A} = \mathbf{L}$$

where

- **L** diagonal matrix of eigenvalues
- **A**: orthonormal matrix of eigenvectors

In R they can be found using `eigen` function

```
## start with the centering matrix
C <- diag(n) - 1/n * rep(1, n) %*% t(rep(1, n)) # centering matrix
Xc <- C %*% X  #centered data
round(colMeans(Xc), 4) # check its' approx 0

##     commun probl_solv    logical      learn   physical appearance
##          0          0          0          0          0          0

S <- t(Xc) %*% Xc / n  #covariance matrix
S

##            commun probl_solv logical  learn physical appearance
## commun     7.3776     0.8512  1.5064 7.4896   6.3312     7.7992
## probl_solv 0.8512     5.6944  2.1368 0.9552   0.9344     0.9104
## logical    1.5064     2.1368  6.0596 1.5944   1.5168     1.5788
## learn      7.4896     0.9552  1.5944 7.8816   6.5752     8.0832
## physical   6.3312     0.9344  1.5168 6.5752   5.6944     6.8504
## appearance 7.7992     0.9104  1.5788 8.0832   6.8504     8.7764

## Doing PCA by matrix functions
spectral <- eigen(S)
spectral$values
```

```
## [1] 29.7582011  7.4672075  3.7076488  0.2868423  0.1467846  0.1173156
```

```
L <- diag(spectral$values)
A <- spectral$vectors
rownames(A) <- rownames(S)
A
```

```
##                   [,1]        [,2]        [,3]         [,4]        [,5]
## commun     -0.49155807  0.08748571  0.01214618 -0.380639251  0.75573635
## probl_solv -0.08675503 -0.69046582  0.71781729  0.008879732  0.01827673
## logical    -0.13662756 -0.70496706 -0.69539380  0.015845890  0.01597971
## learn      -0.50947274  0.08031174  0.02069595 -0.329958740 -0.33064205
## physical   -0.43261611  0.04023081  0.01036964 -0.217845082 -0.56076816
## appearance -0.53428266  0.10274312  0.02196412  0.835735944  0.06699316
##                    [,6]
## commun     -0.185864772
## probl_solv  0.007480667
## logical     0.016594522
## learn       0.717887386
## physical   -0.670223722
## appearance  0.023681484
```

`spectral` returns a list of two objects: `values` (eigenvalues), and `vectors` (matrix of eigenvectors).
Now we can:

1. look at variablity explained by PC (looking at eigenvalue):

   ```
   spectral$value / sum(spectral$value) # percentage explained by each component
   ```

   ```
   ## [1] 0.717341652 0.180002109 0.089375394 0.006914529 0.003538342 0.002827973
   ```

   ```
   cumsum(spectral$value) / sum(spectral$value) # cumulative percentage explained
   ```

   ```
   ## [1] 0.7173417 0.8973438 0.9867192 0.9936337 0.9971720 1.0000000
   ```

   first PC explain 72% while the second the 18%, the last for a small percentage the cumulative; so we can stop at two components (90% of variability)

2. compute the total variance explained by the components

   ```
   sum(spectral$values) # sum of eigenvectors coincides with
   ```

   ```
   ## [1] 41.484
   ```

   ```
   sum(diag(S))         # sum of variances (total variability)
   ```

   ```
   ## [1] 41.484
   ```

3. look at **A** this is the loading matrix (rows variables and columns principal components, we can try to interpret)

```
round(A, 3)

##              [,1]   [,2]   [,3]   [,4]   [,5]   [,6]
## commun     -0.492  0.087  0.012 -0.381  0.756 -0.186
## probl_solv -0.087 -0.690  0.718  0.009  0.018  0.007
## logical    -0.137 -0.705 -0.695  0.016  0.016  0.017
## learn      -0.509  0.080  0.021 -0.330 -0.331  0.718
## physical   -0.433  0.040  0.010 -0.218 -0.561 -0.670
## appearance -0.534  0.103  0.022  0.836  0.067  0.024
```

4. compute the scores

```
head(Y <- X %*% A) # matrix with same dimenson of our original dataset

##           [,1]      [,2]     [,3]      [,4]      [,5]      [,6]
## [1,] -64.87341 -41.84505 25.32417 -15.39198 -30.05441 -1.714282
## [2,] -67.36502 -48.66144 25.47772 -16.03400 -31.33531 -2.216466
## [3,] -66.55825 -43.77018 26.10584 -16.12402 -31.45406 -2.305286
## [4,] -68.35267 -42.07847 24.73539 -16.23449 -31.55929 -2.434767
## [5,] -69.42762 -45.48682 24.09698 -16.54983 -30.71906 -2.555887
## [6,] -69.40433 -38.34110 22.61432 -16.16072 -31.15629 -1.925580
```

for each obs the column are the principal components; when we select a lower number of components we reduce the number of variables

3.12.1.2 Using R functions

To perform principal component analysis there are also functions already implemented in R. These are:

- `prcomp`, that uses function svd on the data matrix.
- `princomp`, that uses function eigen to compute the decomposition of S/R, as we just did

`prcomp` `prcomp` perform PCA using SVD. When using `prcomp`

- `x` is our original dataset (matrix or data.frame); by default the functions center the data
- `scale.` to be set to `TRUE` if we want to work with standardized data too by dividing by (unbiased) standard deviation (default = `FALSE`)

To perform PCA

```
(prcomp_job <- prcomp(X, scale. = FALSE))
```

```
## Standard deviations (1, .., p=6):
## [1] 5.5104910 2.7603622 1.9450746 0.5410141 0.3870144 0.3459911
##
## Rotation (n x k) = (6 x 6):
##                   PC1         PC2         PC3          PC4         PC5
## commun     0.49155807 -0.08748571 -0.01214618  0.380639251 -0.75573635
## probl_solv 0.08675503  0.69046582 -0.71781729 -0.008879732 -0.01827673
## logical    0.13662756  0.70496706  0.69539380 -0.015845890 -0.01597971
## learn      0.50947274 -0.08031174 -0.02069595  0.329958740  0.33064205
## physical   0.43261611 -0.04023081 -0.01036964  0.217845082  0.56076816
## appearance 0.53428266 -0.10274312 -0.02196412 -0.835735944 -0.06699316
##                     PC6
## commun     -0.185864772
## probl_solv  0.007480667
## logical     0.016594522
## learn       0.717887386
## physical   -0.670223722
## appearance  0.023681484

# summary to obtain further prop of variance explained and cumulative

summary(prcomp_job)

## Importance of components:
##                           PC1    PC2     PC3     PC4     PC5     PC6
## Standard deviation     5.5105 2.7604 1.94507 0.54101 0.38701 0.34599
## Proportion of Variance 0.7173 0.1800 0.08938 0.00691 0.00354 0.00283
## Cumulative Proportion  0.7173 0.8973 0.98672 0.99363 0.99717 1.00000
```

returned `prcomp_job` object has:

- `sdev`: square root eigenvalue. Looking at eigenvalues

  ```
  prcomp_job$sdev^2    # eigenvalues

  ## [1] 30.3655113  7.6195995  3.7833151  0.2926963  0.1497802  0.1197098

  spectral$values      # they're a bit different

  ## [1] 29.7582011  7.4672075  3.7076488  0.2868423  0.1467846  0.1173156
  ```

  Eigenvalues are a bit different due to the fact that we computed starting from the biased covariance matrix while *prcomp* use the unbiased covariance matrix

  ```
  spectral$values * n / (n - 1) # exact same results as prcomp

  ## [1] 30.3655113  7.6195995  3.7833151  0.2926963  0.1497802  0.1197098
  ```

- `rotations`: matrix eigenvectors. Results are the same of handmade up to sign changes (in absolute values they're exactly the same)

```
prcomp_job$rotation

##                   PC1         PC2         PC3          PC4         PC5
## commun     0.49155807 -0.08748571 -0.01214618  0.380639251 -0.75573635
## probl_solv 0.08675503  0.69046582 -0.71781729 -0.008879732 -0.01827673
## logical    0.13662756  0.70496706  0.69539380 -0.015845890 -0.01597971
## learn      0.50947274 -0.08031174 -0.02069595  0.329958740  0.33064205
## physical   0.43261611 -0.04023081 -0.01036964  0.217845082  0.56076816
## appearance 0.53428266 -0.10274312 -0.02196412 -0.835735944 -0.06699316
##                     PC6
## commun     -0.185864772
## probl_solv  0.007480667
## logical     0.016594522
## learn       0.717887386
## physical   -0.670223722
## appearance  0.023681484

A

##                   [,1]        [,2]        [,3]         [,4]        [,5]
## commun     -0.49155807  0.08748571  0.01214618 -0.380639251  0.75573635
## probl_solv -0.08675503 -0.69046582  0.71781729  0.008879732  0.01827673
## logical    -0.13662756 -0.70496706 -0.69539380  0.015845890  0.01597971
## learn      -0.50947274  0.08031174  0.02069595 -0.329958740 -0.33064205
## physical   -0.43261611  0.04023081  0.01036964 -0.217845082 -0.56076816
## appearance -0.53428266  0.10274312  0.02196412  0.835735944  0.06699316
##                    [,6]
## commun     -0.185864772
## probl_solv  0.007480667
## logical     0.016594522
## learn       0.717887386
## physical   -0.670223722
## appearance  0.023681484
```

- `x`: it's the matrix of scores $\mathbf{Y}$.

```
## compare with handmade
head(prcomp_job$x)

##             PC1        PC2        PC3        PC4        PC5         PC6
## [1,] -12.096558 -2.5563952 -0.8710214 -1.2643930 -0.7954799  0.47326072
## [2,]  -9.604940  4.2599959 -1.0245741 -0.6223722  0.4854162 -0.02892339
## [3,] -10.411715 -0.6312698 -1.6526974 -0.5323494  0.6041653 -0.11774348
## [4,]  -8.617296 -2.3229729 -0.2822387 -0.4218828  0.7093994 -0.24722444
## [5,]  -7.542345  1.0853742  0.3561619 -0.1065407 -0.1308295 -0.36834431
## [6,]  -7.565630 -6.0603438  1.8388304 -0.4956560  0.3063986  0.26196247
```

```
head(Y)

##           [,1]      [,2]     [,3]      [,4]      [,5]      [,6]
## [1,] -64.87341 -41.84505 25.32417 -15.39198 -30.05441 -1.714282
## [2,] -67.36502 -48.66144 25.47772 -16.03400 -31.33531 -2.216466
## [3,] -66.55825 -43.77018 26.10584 -16.12402 -31.45406 -2.305286
## [4,] -68.35267 -42.07847 24.73539 -16.23449 -31.55929 -2.434767
## [5,] -69.42762 -45.48682 24.09698 -16.54983 -30.71906 -2.555887
## [6,] -69.40433 -38.34110 22.61432 -16.16072 -31.15629 -1.925580

## Here they are really different: prcomp by default centers the data (when we
## did it manually we didn't centere the data). To obtain the same we can just
## center before applying eigenvectors

head(Xc %*% A)              ## ... or

##           [,1]       [,2]       [,3]      [,4]       [,5]        [,6]
## [1,] 12.096558  2.5563952  0.8710214 1.2643930  0.7954799  0.47326072
## [2,]  9.604940 -4.2599959  1.0245741 0.6223722 -0.4854162 -0.02892339
## [3,] 10.411715  0.6312698  1.6526974 0.5323494 -0.6041653 -0.11774348
## [4,]  8.617296  2.3229729  0.2822387 0.4218828 -0.7093994 -0.24722444
## [5,]  7.542345 -1.0853742 -0.3561619 0.1065407  0.1308295 -0.36834431
## [6,]  7.565630  6.0603438 -1.8388304 0.4956560 -0.3063986  0.26196247

head(scale(X, T, F) %*% A) ## ... the same

##           [,1]       [,2]       [,3]      [,4]       [,5]        [,6]
## [1,] 12.096558  2.5563952  0.8710214 1.2643930  0.7954799  0.47326072
## [2,]  9.604940 -4.2599959  1.0245741 0.6223722 -0.4854162 -0.02892339
## [3,] 10.411715  0.6312698  1.6526974 0.5323494 -0.6041653 -0.11774348
## [4,]  8.617296  2.3229729  0.2822387 0.4218828 -0.7093994 -0.24722444
## [5,]  7.542345 -1.0853742 -0.3561619 0.1065407  0.1308295 -0.36834431
## [6,]  7.565630  6.0603438 -1.8388304 0.4956560 -0.3063986  0.26196247
```

- other stuff such as `center` (means), `scale` (logical)

`princomp` `princomp` perform PCA using eigen, as we did by hand. argument of princomp

- the first is the $n \times p$ data matrix
- `cor`, should be set to `TRUE` if the sample correlation matrix is used for PCA and to `FALSE` if the sample covariance matrix is employed.
- if you set `scores=TRUE` (default), then the output will also include an $n \times p$ matrix of principal component scores.

The outcome object is a list of various entries:

- `sdev` gives the standard deviations (the square root of the eigenvalues) of the components
- `loadings` is a matrix with the eigen vectors in the columns (notice that only loadings in modulus larger than 0.1 are printed)
- `center` gives the average vector

```
(princomp_job <- princomp(X, cor = FALSE))

## Call:
## princomp(x = X, cor = FALSE)
##
## Standard deviations:
##    Comp.1    Comp.2    Comp.3    Comp.4    Comp.5    Comp.6
## 5.4551078 2.7326192 1.9255256 0.5355766 0.3831248 0.3425137
##
##  6  variables and  50 observations.

summary(princomp_job) # same stuff as before

## Importance of components:
##                           Comp.1    Comp.2     Comp.3      Comp.4      Comp.5
## Standard deviation     5.4551078 2.7326192 1.92552560 0.535576640 0.383124752
## Proportion of Variance 0.7173417 0.1800021 0.08937539 0.006914529 0.003538342
## Cumulative Proportion  0.7173417 0.8973438 0.98671916 0.993633685 0.997172027
##                             Comp.6
## Standard deviation     0.342513705
## Proportion of Variance 0.002827973
## Cumulative Proportion  1.000000000

## extract the eigenvalues
## -----------------------
princomp_job$sdev^2  # same as manually

##     Comp.1     Comp.2     Comp.3     Comp.4     Comp.5     Comp.6
## 29.7582011  7.4672075  3.7076488  0.2868423  0.1467846  0.1173156

spectral$values      # princomp uses biased version of covariance

## [1] 29.7582011  7.4672075  3.7076488  0.2868423  0.1467846  0.1173156

## matrix of loadings (A)
## -----------------------
princomp_job$loadings # loadings in absolute value < than 0.1 are omitted

##
## Loadings:
##            Comp.1 Comp.2 Comp.3 Comp.4 Comp.5 Comp.6
## commun      0.492                0.381  0.756  0.186
## probl_solv        -0.690  0.718
## logical     0.137 -0.705 -0.695
## learn       0.509                0.330 -0.331 -0.718
## physical    0.433                0.218 -0.561  0.670
## appearance  0.534  0.103        -0.836
##
##                Comp.1 Comp.2 Comp.3 Comp.4 Comp.5 Comp.6
## SS loadings     1.000  1.000  1.000  1.000  1.000  1.000
## Proportion Var  0.167  0.167  0.167  0.167  0.167  0.167
## Cumulative Var  0.167  0.333  0.500  0.667  0.833  1.000

print(princomp_job$loadings, cutoff = 0)

##
## Loadings:
##            Comp.1 Comp.2 Comp.3 Comp.4 Comp.5 Comp.6
## commun      0.492  0.087  0.012  0.381  0.756  0.186
## probl_solv  0.087 -0.690  0.718 -0.009  0.018 -0.007
## logical     0.137 -0.705 -0.695 -0.016  0.016 -0.017
## learn       0.509  0.080  0.021  0.330 -0.331 -0.718
## physical    0.433  0.040  0.010  0.218 -0.561  0.670
## appearance  0.534  0.103  0.022 -0.836  0.067 -0.024
##
##                Comp.1 Comp.2 Comp.3 Comp.4 Comp.5 Comp.6
## SS loadings     1.000  1.000  1.000  1.000  1.000  1.000
## Proportion Var  0.167  0.167  0.167  0.167  0.167  0.167
## Cumulative Var  0.167  0.333  0.500  0.667  0.833  1.000

spectral$vectors

##             [,1]        [,2]        [,3]         [,4]        [,5]         [,6]
## [1,] -0.49155807  0.08748571  0.01214618 -0.380639251  0.75573635 -0.185864772
## [2,] -0.08675503 -0.69046582  0.71781729  0.008879732  0.01827673  0.007480667
## [3,] -0.13662756 -0.70496706 -0.69539380  0.015845890  0.01597971  0.016594522
## [4,] -0.50947274  0.08031174  0.02069595 -0.329958740 -0.33064205  0.717887386
## [5,] -0.43261611  0.04023081  0.01036964 -0.217845082 -0.56076816 -0.670223722
## [6,] -0.53428266  0.10274312  0.02196412  0.835735944  0.06699316  0.023681484

## scores Y
## --------

head(princomp_job$scores)

##          Comp.1     Comp.2     Comp.3     Comp.4     Comp.5      Comp.6
## [1,] -12.096558  2.5563952  0.8710214 -1.2643930  0.7954799 -0.47326072
## [2,]  -9.604940 -4.2599959  1.0245741 -0.6223722 -0.4854162  0.02892339
## [3,] -10.411715  0.6312698  1.6526974 -0.5323494 -0.6041653  0.11774348
## [4,]  -8.617296  2.3229729  0.2822387 -0.4218828 -0.7093994  0.24722444
## [5,]  -7.542345 -1.0853742 -0.3561619 -0.1065407  0.1308295  0.36834431
## [6,]  -7.565630  6.0603438 -1.8388304 -0.4956560 -0.3063986 -0.26196247

head(Y)          # diff because princomp centers the data
```

```
##           [,1]      [,2]     [,3]      [,4]      [,5]      [,6]
## [1,] -64.87341 -41.84505 25.32417 -15.39198 -30.05441 -1.714282
## [2,] -67.36502 -48.66144 25.47772 -16.03400 -31.33531 -2.216466
## [3,] -66.55825 -43.77018 26.10584 -16.12402 -31.45406 -2.305286
## [4,] -68.35267 -42.07847 24.73539 -16.23449 -31.55929 -2.434767
## [5,] -69.42762 -45.48682 24.09698 -16.54983 -30.71906 -2.555887
## [6,] -69.40433 -38.34110 22.61432 -16.16072 -31.15629 -1.925580
```

```
head(Xc %*% A)    # if we do the same we obtain same results as princomp
```

```
##           [,1]       [,2]       [,3]      [,4]       [,5]        [,6]
## [1,] 12.096558  2.5563952  0.8710214 1.2643930  0.7954799  0.47326072
## [2,]  9.604940 -4.2599959  1.0245741 0.6223722 -0.4854162 -0.02892339
## [3,] 10.411715  0.6312698  1.6526974 0.5323494 -0.6041653 -0.11774348
## [4,]  8.617296  2.3229729  0.2822387 0.4218828 -0.7093994 -0.24722444
## [5,]  7.542345 -1.0853742 -0.3561619 0.1065407  0.1308295 -0.36834431
## [6,]  7.565630  6.0603438 -1.8388304 0.4956560 -0.3063986  0.26196247
```

3.12.1.3 Choosing number of principal components

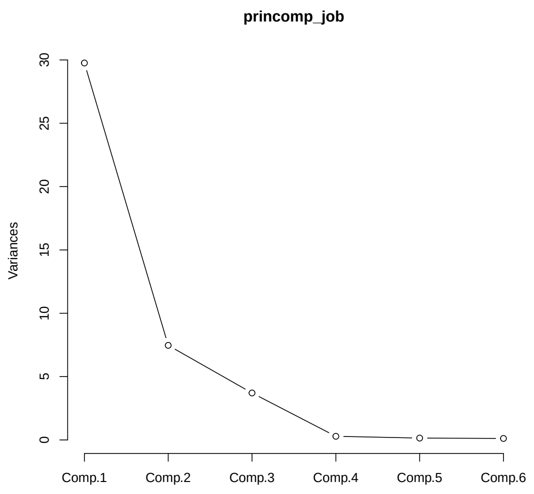
Cumulative proportion of variance explained This approach suggests to choose as many principal components as are needed to explain approximately 80-90% of the total variance. Therefore, in this case the number of PCs needed is 2.

```
cumsum(spectral$value) / sum(spectral$value) # cumulative percentage explained
```

```
## [1] 0.7173417 0.8973438 0.9867192 0.9936337 0.9971720 1.0000000
```

Screeplot The *scree plot* is a plot of l_k against k $(k = 1, \dots, p)$. Usually, the curve tends to become flat after a sharp decline. The flat portion corresponds to noise components, that are not able to capture the leading variability. Therefore, the criterion suggests to retain a number of components equal to the value of k at which the elbow of the scree plot occurs. According to this criterion, the number of PCs to be selected here would be 3 (comp4, 5, 6 are flat).

```
plot(princomp_job, type = "lines")
```



```
spectral$values # last three are close to zero

## [1] 29.7582011  7.4672075  3.7076488  0.2868423  0.1467846  0.1173156
```

Kaiser's rule According to this criterion, the number of principal components to retain is the number of components whose variance is higher than the average variance. Thus, in this case the solution is 2.

```
princomp_job$sdev^2 > mean(princomp_job$sdev^2) # the first two component are selecte

## Comp.1 Comp.2 Comp.3 Comp.4 Comp.5 Comp.6
##   TRUE   TRUE  FALSE  FALSE  FALSE  FALSE
```

3.12.1.4 Interpretation of loadings

We choos to work with 2 PC, we can try to interpret it focusing on loadings

```
princomp_job$loadings[, 1:2] # matrix eigenvectors, first two columns

##                Comp.1      Comp.2
## commun     0.49155807  0.08748571
## probl_solv 0.08675503 -0.69046582
## logical    0.13662756 -0.70496706
## learn      0.50947274  0.08031174
## physical   0.43261611  0.04023081
## appearance 0.53428266  0.10274312
```

In the table above:

- first PC (that accounts for about the 72% of the total variability) all the loadings but `probl_solv` and `logical` (which are close to zero) have the same size and almost the same magnitude. Hence, this component appears to be a sort of average of the measurements.

- In the second PC the only two loadings that are not close to zero are those related to the logical ability and problem solving. Therefore it separates police officers with a marked logical skill (with a small score on the test, as the magnitude is negative) from the others.

Alternatively, it is possible to interpret PCs by evaluating the correlations between each principal component and all the observed variables, i.e:

$$\mathrm{Corr}\,(y_1, \mathbf{x}) = l_1^{1/2}\mathbf{a}_1^T\mathbf{D}^{-1/2}$$
$$\mathrm{Corr}\,(y_2, \mathbf{x}) = l_2^{1/2}\mathbf{a}_2^T\mathbf{D}^{-1/2}$$

where $\mathbf{D}$ is the diagonal matrix containing the original variances.

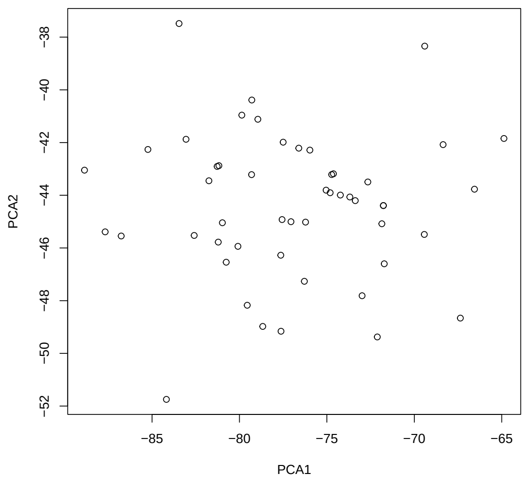
```
## we need to compute D
D <- diag(diag(S))

# Applying the formula above, for the first principal component
# sqrt(l1)                *  a_1^T          D^{-1/2}
sqrt(spectral$values[1]) * t(A[, 1])   %*% solve(D^0.5)

##            [,1]       [,2]       [,3]       [,4]       [,5]       [,6]
## [1,] -0.9872352 -0.1983234 -0.3027748 -0.9899587 -0.9889676 -0.9838213

# or just by cor  is the samme
cor(Y[, 1], X)

##          commun probl_solv    logical      learn   physical appearance
## [1,] -0.9872352 -0.1983234 -0.3027748 -0.9899587 -0.9889676 -0.9838213

## similar thing for the second
spectral$values[2]^0.5 * t(A[, 2])   %*% solve(D^0.5)

##            [,1]       [,2]      [,3]       [,4]       [,5]       [,6]
## [1,] 0.08801541 -0.7906737 -0.782575 0.07817195 0.04606954 0.09477061

cor(Y[, 2], X)

##          commun probl_solv   logical      learn   physical appearance
## [1,] 0.08801541 -0.7906737 -0.782575 0.07817195 0.04606954 0.09477061
```

The first principal component is highly negatively related with all the observed variables except for `probl_solv` and logical. Thus, all variables contribute more or less in the same way to the first principal component, confirming the interpretation given above. The second principal component is highly negatively correlated with `l_solv` and `logical`; thus, it separates police officers with a marked logical skill (with a small score on the test, as the magnitude is negative) from the others.

3.12.1.5 Visualization of PC

Since we have just two components we can visualize them. The object scores is a matrix 50×2 containing the scores of the units with respect to the first two principal components.

```
plot(Y[, 1], Y[ , 2], xlab = "PCA1", ylab = "PCA2")
```



3.12.1.6 Are all the units well represented by the bi-dimensional plot?

As the bi-dimensional plot is just an approximation of the structure in the original p-dimensional space, it may happen that not all of the n statistical units are well represented in the bi-dimensional projection.
A way to check the adequacy of the approximation for each statistical unit is an inspection of the scores on the last (discarded) PCs. In particular, if a unit has high scores on the last PCs, this means that it is largely displaced when projected on the PC plane, i.e. it is misrepresented.
One could consider, for each statistical unit, the sum of the squared scores on the last $p - m$ PCs. The position on the PC plane of those units having a large value of such a sum should be carefully considered.

```
(d <- apply(Y[, 3:6], 1, function(x) sum(x^2)))

##  [1] 1784.433 1893.018 1936.171 1877.315 1804.755 1746.998 1684.826 1743.272
##  [9] 1880.757 1915.520 1880.757 1681.001 1854.007 1668.917 1964.539 1859.880
## [17] 1727.699 1865.102 1759.574 2104.255 1863.209 1873.058 2184.831 1703.492
## [25] 1707.550 1831.796 1938.200 1732.942 1830.631 1912.833 1741.321 1780.767
## [33] 1745.660 1921.742 1795.591 1862.057 1854.136 1722.972 1894.969 1891.101
## [41] 1756.409 1970.561 1901.513 1819.324 1868.010 1812.201 1717.760 1811.706
## [49] 1900.057 1828.348
```

Since these values are high, it is possible to conclude that the first two PCs are not enough to well represent this dataset.
We can find the observations that are represented the worst using the `order` function.

```
head(d_order <- order(d, decreasing=TRUE)) # these are the worst represented

## [1] 23 20 42 15 27  3

job[d_order[1:5], ]

##    commun probl_solv logical learn physical appearance
## 23     18         59      20    50       54         20
## 20     17         57      20    49       54         20
## 42     20         56      22    53       56         24
## 15     16         55      22    49       53         19
## 27     18         57      24    51       54         21
```

3.12.2 Sparrows dataset

Now we do the same for the `sparrow` dataset (but we use correlation instead of covariance matrix). In February 1898, there was a severe winter storm with rain, sleet, and snow near Providence, RI (Rhode Island). 136 English sparrows were found freezing and brought to Dr. Bumpus' laboratory at Brown University. Of those, 72 survived and 64 died. Bumpus took advantage of the opportunity to study an episode of natural selection. He measured a number of characteristics of the birds and analyzed them to find differences between the survivors and those that perished. Here we consider a sample of 49 sparrows. The dataset sparrows.dat contains the following variables:

- `totL`: total length
- `AlarE`: alar extent
- `bhL`: length of beak and head
- `hL`: length of humerus
- `kL`: length of keel of sternum

```
sparrows <- read.table("multivariate_statistics/data/sparrows.dat", header = TRUE)

## Warning in file(file, "rt"):  non è possibile aprire il file ’multivariate_statistics/data/s
File o directory non esistente
## Error in file(file, "rt"):  non è possibile aprire la connessione

head(sparrows)

## Error:  oggetto ’sparrows’ non trovato

summary(sparrows)

## Error:  oggetto ’sparrows’ non trovato
```

```
(R <- cor(sparrows)) # correlations are high so it makes sense

## Error:  oggetto 'sparrows' non trovato
```

Is PCA justified Since the correlation values look quite large, in this context PCA seems to be useful in order to reduce dimensionality.

```
# decide to work with covariance or correlation
sapply(sparrows, var)

## Error:  oggetto 'sparrows' non trovato

## we have different magnitudes of variances: the first two variables takes
## values that are large, while last three have different units of
## measuremente.  so we standardize data (and use covariance matrix) or use
## directly correlation matrix.
```

Decide between covariance and correlation Moreover, since in this example variances are very different, it is advisable to use the correlation matrix to carry out the PCs. This is equivalent to perform the PCA on the covariance matrix of the standardized data.

Using matrix functions Principal Components can be derived from the spectral decomposition of the correlation matrix by using the `eigen` function.

```
spectral <- eigen(R)
spectral$values # eigevalues

## [1] 4.03516605 1.26093572 0.63059444 0.03460586 0.02232708 0.01637085

A <- spectral$vectors # eigevectors
rownames(A) <- rownames(R)
A

##            [,1]        [,2]        [,3]         [,4]         [,5]          [,6]
## [1,] -0.4898867  0.10661812 -0.01931189 -0.335344756  0.677694372  0.4201724803
## [2,] -0.1111630 -0.72089324 -0.68377657  0.008701665  0.018150128 -0.0004383121
## [3,] -0.1636455 -0.66488745  0.72831261  0.015284637  0.019952761 -0.0085914040
## [4,] -0.4913118  0.09769660 -0.02568178 -0.262692420  0.009760144 -0.8242001751
## [5,] -0.4920224  0.06977629 -0.01668897 -0.266769473 -0.733753782  0.3784259095
## [6,] -0.4872378  0.11161019 -0.02644446  0.864327077  0.038896332  0.0294785507
```

To compute the PCA scores, in order to obtain the same result as `princomp`, x should be scaled

```
head(scores <- as.matrix(sparrows) %*% A)

## Error:  oggetto 'sparrows' non trovato
```

```
head(scores_stand <- scale(sparrows, T, T) %*% A) # to get same results as princomp we scale

## Error:  oggetto 'sparrows' non trovato
```

Compute the importance of each component in explaining the total variance

```
# proportion explained
spectral$values / sum(spectral$values) # prop explained

## [1] 0.672527675 0.210155954 0.105099073 0.005767644 0.003721180 0.002728475

cumsum(spectral$values) / sum(spectral$values) # first two components are enough

## [1] 0.6725277 0.8826836 0.9877827 0.9935503 0.9972715 1.0000000

# total variability: is number of variables working with std data the varainces
# is 1)
sum(spectral$values)

## [1] 6

sum(diag(R))

## [1] 6
```

We find that the first PC accounts for the 72.3% of the total variation, whereas the first two components cover about the 83% of the total variability. Notice that the sum of the eigenvalues is equal to the number of variables as the variance of each standardized variable is 1.

Using `princomp` on correlation matrix Here we use `cor=TRUE`, so princpomp know it has to standaridze the data

```
pca_s <- princomp(sparrows, cor = TRUE, scores=TRUE)

## Error:  oggetto 'sparrows' non trovato

## eigenvalues
## -----------
pca_s$sdev^2     # are the

## Error:  oggetto 'pca_s' non trovato

spectral$values #  same

## [1] 4.03516605 1.26093572 0.63059444 0.03460586 0.02232708 0.01637085

## eigenvectors
## -----------
print(pca_s$loadings, cutoff = 0)    # same up to sign

## Error:  oggetto 'pca_s' non trovato
```

```
spectral$vectors # change (see the uper matrix)

##              [,1]        [,2]        [,3]         [,4]         [,5]          [,6]
## [1,] -0.4898867  0.10661812 -0.01931189 -0.335344756  0.677694372  0.4201724803
## [2,] -0.1111630 -0.72089324 -0.68377657  0.008701665  0.018150128 -0.0004383121
## [3,] -0.1636455 -0.66488745  0.72831261  0.015284637  0.019952761 -0.0085914040
## [4,] -0.4913118  0.09769660 -0.02568178 -0.262692420  0.009760144 -0.8242001751
## [5,] -0.4920224  0.06977629 -0.01668897 -0.266769473 -0.733753782  0.3784259095
## [6,] -0.4872378  0.11161019 -0.02644446  0.864327077  0.038896332  0.0294785507

## prop variance explained
## -----------
summary(pca_s)

## Error:  oggetto 'pca_s' non trovato
```

Regarding **Y** there is a slight difference between the two results; this is due to the fact that scale uses unbiased variances to standardize, while `princomp` does not!

```
## Y
## --
head(pca_s$scores) # princomp computes the scores after centering and scaling x

## Error:  oggetto 'pca_s' non trovato

head(scores) # without standardizing data they're vastly different

## Error:  oggetto 'scores' non trovato

# with standardization: equal to pca_s$scores up to a sign change!
head(scores_stand) # standardizing using unbiased covmatrix

## Error:  oggetto 'scores_stand' non trovato
```

The final standardized score are actually similar but not equivalent to those returned by `princomp` stored in `pca_s` (some decimals are changed): the reason is that `scale` use the unbiased covariance matrix, while `princomp` uses the biased ones.
To get the exactly what with `princomp` does:

```
n <- nrow(sparrows)

## Error:  oggetto 'sparrows' non trovato

C <- diag(n) - 1/n * rep(1, n) %*% t(rep(1, n)) # centering matrix
Xc <- C %*% as.matrix(sparrows)  #centered data

## Error:  oggetto 'sparrows' non trovato

S <- 1/n * t(Xc) %*% Xc
D <- diag(diag(S))
Z <- Xc %*% solve(D^0.5)
```

```
scores_z <- Z %*% A
scores_z[1:5, ] # now exactly equivalent up to sign changes to

##          [,1]       [,2]       [,3]       [,4]        [,5]         [,6]
## [1,] 4.593657  0.9260852 -0.3843684 0.46840774  0.33965785 -0.047771308
## [2,] 3.440966 -1.8416263 -0.3608873 0.20053062 -0.19328148 -0.042553546
## [3,] 3.846632  0.1450697 -0.6847236 0.16475441 -0.24852154 -0.028041971
## [4,] 3.213781  0.8902318 -0.1438149 0.12039210 -0.30511080  0.001972478
## [5,] 2.740818 -0.4850129  0.1635882 0.02285044 -0.01607894  0.145827499

pca_s$scores[1:5, ]

## Error:  oggetto 'pca_s' non trovato
```

Select n of components According to this criterion we should retain as many principal components as are needed to explain approxi- mately 80-90% of the total variance. Thus, in this case the number of PC needed is 2.

```
summary(pca_s) # two principal components

## Error:  oggetto 'pca_s' non trovato
```

According to this criterion, the number of PCs to be selected here would be 2.

```
plot(pca_s, type="l") # screeplot here seems that two components are enough

## Error:  oggetto 'pca_s' non trovato
```

The Kaiser's rule for PCs derived from a correlation matrix suggests to retain only those components that exhibit eigenvalues of R larger than 1. The motivation underlying this rule is that we want to retain all the principal components that have a variance larger than the one related to the original variables (that is equal to 1 for standardized data). In this case only the first Principal Component should be used.

```
pca_s$sdev^2 >mean(pca_s$sdev^2) # just the first

## Error:  oggetto 'pca_s' non trovato
```

Interpretation of loadings Taking the first two components . . .

```
# --------------
# interpretation
# --------------
pca_s$loadings[ , 1:2]

## Error:  oggetto 'pca_s' non trovato
```

In the first PC (that accounts for about the 72% of the total variability) all the loadings have the same size and almost the same magnitude. Hence, this component appears to be a sort of average size of the sparrows. Even if the second PC is not important in recovering a reduced dimension representation of our data, we can try to give it an empirical meaning. Specifically, It appears to be a linear contrast as some variables have a positive coefficient and some others have a negative one. It separates sparrows having a small alar extent and short humerus, a small beak and a large keel of sternum from all the others. Therefore, it can be thought of as a measure of shape. The first loading is close to zero so it is not interpretable. The same result can be obtained by analyzing the correlations between each PC and all the observed variables:

```
## first component
spectral$values[1]^0.5  *  t(A[, 1]) %*% solve(diag(diag(R))^0.5)

##            [,1]       [,2]       [,3]       [,4]       [,5]       [,6]
## [1,] -0.9840708 -0.2233011 -0.3287266 -0.9869336 -0.9883609 -0.9787497

cor(scores_stand[, 1], X) # same result

## Error:  oggetto 'scores_stand' non trovato

## second component
spectral$values[2]^0.5  *  t(A[, 2]) %*% solve(diag(diag(R))^0.5)

##           [,1]       [,2]       [,3]      [,4]       [,5]      [,6]
## [1,] 0.119723 -0.8095011 -0.7466114 0.1097049 0.07835277 0.1253286

cor(scores_stand[, 2], X) # same result

## Error:  oggetto 'scores_stand' non trovato
```

The first principal component is highly negatively correlated with each of the observed variables. All variables contribute more or less in the same way to the first principal component, confirming the interpretation given above. The second principal component is negatively correlated with AlarE, bhL, hL and positively related with kL, separating sparrows having a small alar extent and short humerus, a small beak and a large keel of sternum from all the others.

Plotting of first two components The object scores is a matrix 49×2 containing the scores of the units with respect to the first two principal components.

```
plot(scores_stand[, 1], scores_stand[, 2])

## Error:  oggetto 'scores_stand' non trovato
```

Are all the units well represented by the bi-dimensional plot? Notice that the sligth difference below are due to the reason explained before, i.e. `scale` uses corrected variances to standardize, while princomp not!

```
apply(pca_s$scores[, -(1:2)], 1, function(x) sum(x^2))    # biased std

## Error:  oggetto 'pca_s' non trovato

(d <- apply(scores_stand[, -(1:2)], 1, function(x) {sum(x^2)})) # correct std

## Error:  oggetto 'scores_stand' non trovato

sort(d, decreasing =TRUE)

##  [1] 2184.831 2104.255 1970.561 1964.539 1938.200 1936.171 1921.742 1915.520
##  [9] 1912.833 1901.513 1900.057 1894.969 1893.018 1891.101 1880.757 1880.757
## [17] 1877.315 1873.058 1868.010 1865.102 1863.209 1862.057 1859.880 1854.136
## [25] 1854.007 1831.796 1830.631 1828.348 1819.324 1812.201 1811.706 1804.755
## [33] 1795.591 1784.433 1780.767 1759.574 1756.409 1746.998 1745.660 1743.272
## [41] 1741.321 1732.942 1727.699 1722.972 1717.760 1707.550 1703.492 1684.826
## [49] 1681.001 1668.917
```

Since these values are low, it is possible to conclude that the first two PCs are enough to well represent this dataset.

Capitolo 4

Factor analysis

4.1 Introduction

Thus method was invented by Spearman (psycometrician) in 1904 to measure intelligence (Galton wanted to study correlation of intelligence between father and sons; but measure of intelligence was not available so he measured height, something measurable).

Intelligence is a latent variable: it's not observed (as all psychological variables are).

Spearman had this dataset on students on performance of students in three subjects' test: X_1 classics, X_2 french and X_3 english with correlation matrix

$$\rho = \begin{bmatrix} 1 & 0.83 & 0.78 \\ & 1 & 0.67 \\ & & 1 \end{bmatrix}$$

Variables are positive correlated (and pretty high correlation).

- I observe positive and high correlation: does it mean that these variables are correlated because of another varaible which drives the correlation?
- if i condition /eliminate on the unobserved variable can I diminish the correlation of the observed (in this case the correlation is due to the hidden variable). It's the same of partial corrrelation but with a variable which is not observed

Two appreciable differences of factor analysis with respect to PCA:

- what spearman did was to figure out *a model* which could explain the observed correlation: any model require *assumptions* (while in PCA we had no theoretical assumptions);
- the focus here is to explain *correlation* (off diagonal elements of variance/covariance/correlation matrix), while in PCA was on variance (in diagonal elements)

So is there a latent variable that allows to explain the observed correlation? Spearman assumed that the performance (random variables on single students) is composed as

$$X_1 = \lambda_1 f + u_1$$

where[1]:

- X_1, X_2 and X_3 are the *observed variables* (grades).
- λ_1, λ_2 and λ_3 are known as *factor loadings*
- the quantity f has no subscript so it is the same for all the variables: its called *common factor*
- the $u_1, \ldots, u_3$ are different for each variables and are known as *unique factors*

The idea that Spearman had was:

- I have a given level of intelligence f (which is a random variable)
- my result in classics (X_1) is due to my intelligence (weighed by a contribution λ_1: λ_1 is fixed, not related to the single unit
- then there is u_1, a random variable (like f) which takes into account all other factors impacting performance in classics other than intelligence. This is like ε term in regression: it's random variablity around the model.

Some considerations:

- If data have been generated in this way I can explain the correlation between observed variales ($X_1, \ldots, X_3$):
- this model above looks like a regression model, but is different becaus all what we see on the right side of $=$ is unknown while in regression is all available

After posing the model, spearman research opened big debate: people started to put question regarding intelligence: is there a unique intelligence? actually no, there are different side of intelligence, which is a good motivating example for introducing the the general model of intelligence, a generalization of the one above, applying a general linear factor model, in which a generic test X_i can be explained in terms of m intelligence components

$$X_i = \lambda_{i1} f_1 + \lambda_{i2} f_2 + \ldots + \lambda_{ik} f_k + \ldots \lambda_{im} f_m + u_i$$

where

- we have many f for differnt kind of intelligence
- the weights/loadings lambdas has two subscript, the first concerning the explained/observed variable, the second the latent/intelligence one varaible)

[1]Again for every topic the notation changes (λ here has nothing to do with lamdba of PCA)

This factor model can be written in matrix form (considering all the p tests to be explained for a single unit) as

$$\underset{p\times 1}{\mathbf{X}} = \underset{p\times m}{\Lambda}\underset{m\times 1}{f} + \underset{p\times 1}{\mu}$$

where:

- the matrix $\mathbf{\Lambda}$ is the *factor loading matrix* ($p \times m$ because of p observed variables and m latent ones)
- $\mathbf{f}$ is the vecctor of *common factors*
- $\mathbf{u}$ is the vector of *unique factors*

Again we are in a single unit (with p observed variables to be explained) not a sample of units.
The matrix Lambda will be:

$$\mathbf{\Lambda} = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \dots & \lambda_{1k} & \dots & \lambda_{1m} \\ \dots \\ \lambda_{i1} & \lambda_{i2} & \dots & \lambda_{ik} & \dots & \lambda_{im} \\ \dots \\ \lambda_{p1} & \lambda_{p2} & \dots & \lambda_{pk} & \dots & \lambda_{pm} \end{bmatrix}$$

Again all what appears on the right hand side of $=$ is unknown: in order to be able to estimate the model we need to put constraints on the parameters/the unknown random variables/vector (f and u).[2]

4.2 Assumptions

We have the following assumptions: the first twos are just symplyfing while the last two are the most important:

1. we assume to work with 0 centered random variables, that is

$$\mathbb{E}[\mathbf{f}] = \mathbf{0} \quad \mathbb{E}[\mathbf{u}] = \mathbf{0}$$

This is a low-cost simplyfing assumption; result can be easily obtained by working on mean centered observations.
If I had not been working with mean center obs

TODO: check 11

$$X_1 = \mu_i + \lambda_{i1} f_1 + \lambda_{im} f_m$$

but this complicate the model and adds nothing

$$\underbrace{E(X_1)}_{E(X_1-\mu_1)=0} = \lambda_1 \underbrace{\mathbb{E}[f_1]} = 0 + \dots \lambda_{im} \underbrace{Ef_m}_{=0} + \underbrace{Eu}_{=0}$$

[2]When we estimate a model, to estimate we always make assumptions: eg in regression epsilon has 0 mean, constant variance and uncorrelated between obs. We need similar conditions here, but on $\mathbf{f}$ and $\mathbf{u}$ (while in regression was only on ε)

2. variance covariance matrix of latent variables is identity

$$E(ff^T) = V(f) = I_m$$

The first is the variance covariance matrix of **f** since **f** is mean centered. This means that we assume that the common factors are assumed to have unit varaince and to be uncorrelated
This again is a simplyfiny assumptions: its not necessarily but it can be proved (using Choleski decomposition) that any model can be transformed to a model respecting this condition

3. this is a new fondamental condition

$$\begin{aligned} \mathbb{E}\left[\mathbf{f}\mathbf{u}^T\right] &= \underset{m\times p}{\mathbf{0}} \\ \mathbb{E}\left[\mathbf{u}\mathbf{f}^T\right] &= \underset{p\times m}{\mathbf{0}} \end{aligned}$$

these are null matrices of different sizes: actually these are are the variance/covariance between f and u so $\text{Cov}(\mathbf{f}, \mathbf{u}) = \mathbf{0}$. These tells us that **common factors and the unique factors are uncorrelated**.
Eg there's no correlation between intelligence and other aspect/noise that impact on performance of a score

4. finally

$$\mathbb{E}\left[\mathbf{u}\mathbf{u}^T\right] = \text{Var}\left[u\right] = \mathbf{\Psi}$$

with $\mathbf{\Psi}$ a diagonal matrix such as

$$\mathbf{\Psi} = \begin{bmatrix} \psi_{11} & & 0 \\ 0 & \psi_{ii} & 0 \\ 0 & & \psi_{pp} \end{bmatrix}$$

This last assumption is that the unique factors are uncorrelated among them (so other things influencing my performance on classics are not correlated with other things influencing my performance in math).
These variances ψ_{ii} are called **uniquenesses** or **specific variances**: so we have specific/different variances for each factor

TODO: CHECK

Now assuming that all those conditions are met/hold, we're able to compute, as a consequence of the conditions the covariance between the observed variables as

$$\begin{aligned} \mathbb{E}\left[XX^T\right] \overset{(0)}{=} \Sigma &= \mathbb{E}\left[(\mathbf{\Lambda f} + \mathbf{u})(\mathbf{\Lambda f} + \mathbf{u})^T\right] \\ &= \mathbb{E}\left[\mathbf{\Lambda f f}^T\mathbf{\Lambda}^T + \mathbf{\Lambda f u}^T + \mathbf{u f}^T\mathbf{\Lambda}^T + \mathbf{u u}^T\right] \\ &\overset{(1)}{=} \mathbf{\Lambda}\,\mathbb{E}\left[\mathbf{f f}^T\right]\mathbf{\Lambda}^T + \mathbf{\Lambda}\,\mathbb{E}\left[\mathbf{f u}^T\right] + \mathbb{E}\left[\mathbf{u f}^T\right]\mathbf{\Lambda}^T + \mathbb{E}\left[\mathbf{u u}^T\right] \\ &\overset{(2)}{=} \mathbf{\Lambda\Lambda}^T + \mathbf{\Psi} \end{aligned}$$

where in

- (0) the expected value is still covarince matrix becacuse dealing with mean centered data (so Σ)

- (1) we split the expected value; Λ are constant and can be put outside expectation

- (2) we substituted $\mathbb{E}\left[\mathbf{f} f^T\right] = \mathbf{I}$ (for assumption 2), $\mathbb{E}\left[\mathbf{fu}^t\right] = \mathbf{0}$ and $\mathbb{E}\left[\mathbf{uf}^t\right] = \mathbf{0}$ (for assumption 3) and $\mathbb{E}\left[\mathbf{uu}^T\right] = \mathbf{\Psi}$

Thus if the factor model holds, Σ (the covaraince matrix of observed variables)

- is $= \Lambda\Lambda^T + Psi$

- as $\mathbf{\Psi}$ is diagonal, this means that the observed covarainces (off diagonal elements in Σ) are completely determined/accounted for/by the common factors

This means that if a model like the one holds, than we can explain correlation using only factors (since the remaining Ψ is diagonal).

TODO: CHECK

Remark 23. Recappino:

- Factor analysis ($X = \mathbf{\Lambda f} + \mathbf{u}$) is a linear model aimed at explaining *observed* correlation (between observed variables)

- $\mathbf{u}$ has the same role of residual ε in linear models

- as in PCA this model perform dimension reduction: observed variables are p while latent factors are m which is expected to be smaller than p

- specific elements of this model is that all what is on the rhs is unknown/unobserverd (different from linear models where ε is the only unknown/random)

- in order to obtain estimates we need to put constraints on f, u and on their relationship. The first assumption eases the estimation of a simpler model without loss of generality; the second assumption is not fundamental (we will relax it); always possible to transform a model without to a model enforcing this

- if the data are generated under the factor model then we can write Σ as linear combination of Λ and Ψ. Very important that $\mathbf{\Psi}$ is diagonal to say that there's no residual correlation

Given our assumptions on f and u we obtain that if the data have been generated according to model $\mathbf{X} = \mathbf{\Lambda f} + \mathbf{u}$, then $\mathbf{\Sigma} = \mathbf{\Lambda\Lambda}^T + \mathbf{\Psi}$. So to expand a bit

$$\Sigma = \mathbf{\Lambda\Lambda}^T + \mathbf{\Psi}$$

$$\begin{bmatrix} \sigma_1^2 & \sigma_{12} & \dots & \sigma_{1p} \\ & \sigma_{22} & \dots & \sigma_{2p} \\ & & \sigma_i^2 & \sigma_{ip} \\ & & & \sigma_p^2 \end{bmatrix} = \begin{bmatrix} \lambda_{11} & \dots & \lambda_{1k} & \dots & \lambda_{1n} \\ \dots \\ \lambda_{i1} & \dots & \lambda_{ik} & \dots & \lambda_{in} \\ \dots \\ \lambda_{p1} & \dots & \lambda_{pk} & \dots & \lambda_{pn} \end{bmatrix} \begin{bmatrix} \lambda_{11} & \dots & \lambda_{i1} & \dots & \lambda_{p1} \\ \dots \\ \lambda_{1k} & \dots & \lambda_{ik} & \dots & \lambda_{pk} \\ \dots \\ \lambda_{1n} & \dots & \lambda_{in} & \dots & \lambda_{pn} \end{bmatrix} + \begin{bmatrix} \psi_{11} & 0 & 0 \\ 0 & \psi_{ii} & 0 \\ 0 & 0 & \psi_{pp} \end{bmatrix}$$

Now let's focus on generic element σ_i^2 of Σ it's generated considering the i-th row of $\mathbf{\Lambda}$ and i-th column of $\mathbf{\Lambda}^T$ (and the eleemnt ii of Ψ). So we have

$$\sigma_i^2 = \underbrace{\sum_{k=1}^{m} \lambda_{ik}^2}_{h_i^2} + \psi_{ii} = \lambda_{i1}^2 + \ldots + \lambda_{ik}^2 + \ldots + \lambda_{in}^2 + \psi_{ii}$$

so if the factor model holds, the **observed variance can be decomposed** to part due to the components/lambda variables (common part) and part due to psi (unique part) The quantity:

TODO: cHECK

- $h_i^2 = \sum_{k=1}^m \lambda_{ik}^2$ is called *communality*. the communality is the part of the observed variance that is accounted for by the common factor
- ψ_{ii} the uniqueness: the uniqueness is related to the specific/unique factor

So we can say that the observed variance can be decomposed in the sum of communality + uniqueness.
The latent variables are able to explain just a part of the observed variablity then there's the specific part off course

Focusing on the off diagonal elements, say σ_{ip} this is obtained multiplying the i-th row of $\mathbf{\Lambda}$ and p-th, last column, thus

$$\sigma_{ip} = \sum_{k=1}^{m} \lambda_{ik}\lambda_{pk} + 0$$

(at the end added 0 because off diagonale element of $\mathbf{\Psi}$, $\psi_{ip} = 0$) so here if the model holds, all the observed covariance are fully explained by the observed covariances

TODO: in general CHECK

4.3 Factor loading matrix

Let's focus on $\mathbf{\Lambda}$: we've said that it is the factor loading matrix. What does this mean?
In the first row we have the contribution of each common factor to variable X_1. It tells how much each factor "loads" to obtained the observed variables (look at the model in extended form); it might be that not all the factor are relevant for a certain observed variable.

Now let's derive the expected value of

$$\mathbb{E}\left[\mathbf{X}\mathbf{f}^T\right] = \text{Cov}\left(\mathbf{X}, \mathbf{f}\right)$$

this is the covariance (as alla the variables have zero mena) between the observed variable $\mathbf{X}$ and the common factor $\mathbf{f}$. If $\mathbf{X} = \mathbf{\Lambda}\mathbf{f} + \mathbf{u}$, then the expected value above, to apply the definition

$$\begin{aligned}
\mathbb{E}\left[\mathbf{X}\mathbf{f}^T\right] &= \mathbb{E}\left[(\mathbf{\Lambda}\mathbf{f} + \mathbf{u})\mathbf{f}^t\right] \\
&= \mathbb{E}\left[\mathbf{\Lambda}\mathbf{f}\mathbf{f}^T + \mathbf{u}\mathbf{f}^T\right] \\
&\overset{(1)}{=} \mathbf{\Lambda}\underbrace{\mathbb{E}\left[\mathbf{f}\mathbf{f}^T\right]}_{\mathbf{I}} + \underbrace{\mathbb{E}\left[\mathbf{u}\mathbf{f}^T\right]}_{\mathbf{0}} \\
&= \mathbf{\Lambda}
\end{aligned}$$

where in

- (1) we take out Λ (which acts as constant)
- (2) we substitute from assumptions $\mathbb{E}\left[\mathbf{uf}^T\right] = \mathbf{I}$ and $\mathbb{E}\left[\mathbf{uf}^T\right] = \mathbf{0}$

So beside being the factor loading matrix, Λ is *also the covariance matrix between observed variable X and latent/common factor* $\mathbf{f}$.

4.4 Equivariance

The linear factor model is equivariant with respect to scale changes Assume that

$$\mathbf{Y} = \mathbf{CX}$$

where C is a scale change matrix which is square and diagonal: so we change unit by premultipling our variable by the matrix $\mathbf{C}$ (we multiply each column of X by a constant). It turns out that:

$$\mathbf{Y} = \mathbf{CX} = C(\Lambda_X f + u) = \underbrace{C\Lambda_X}_{\Lambda_Y} f + Cu = \Lambda_Y f + Cu$$

I have a new factor model with the same common factor f, but the lambda matrix has been rescaled. $\mathbf{\Lambda_Y}$ is the original but rescaled applying $\mathbf{C}$ The new factor loading matrix is the old factor loading matrix times the scale change. This proves that linear factor model is scale equivariant. **TODO**: CHECK
If we rescale we don't need to refit the model but just multiply the factor loadings for the matrix of $\mathbf{C}$.

What happens to variance of Y?

$$\begin{aligned}\operatorname{Var}[\mathbf{Y}] &= \mathbf{C}\operatorname{Var}[\mathbf{X}]\,\mathbf{C}^T \overset{(1)}{=} \mathbf{C}\Sigma\mathbf{C} = C(\Lambda_X\Lambda_X^T + \Psi_X)C \\ &= C\Lambda_X\Lambda_X^T C + C\Psi_X C\end{aligned}$$

where in substitution (1) we removed transposition from $\mathbf{C}$ since it's symmetric. So the same happens with variance: we don't need to reestimate but just take the estimate from X and, if we assume that as transformation we take the standardizing matrix ($1/\sqrt{\sigma}$ you know)

$$C = \Delta^{-1/2}$$

and define

$$Y = \Delta^{-1/2} X$$

Y are standardized variable because have zero mean but also unitary variance/sd

$$\Lambda_Y = \Delta^{-1/2}\Lambda_X$$

This means that the factor loading matrix referred to the standardized variables is equal to the factor loading matrix of the raw data multiplied by $\Delta^{-1/2}$

Interesting: we can model on the unstandardized data and go in the model with standardized variable by just preapplying

TODO: CHECK

So either i premultiply by $\Delta^{-1/2}$ to go to the std data or $\Delta^{1/2}$ to the unstandardized data.
This is not the case with PCA

we can always move from the solution on the original data to the one on the standardized data by just performing a simple scale change (with $\Delta^{-1/2}$)

what is Λ_Y? as

$$\Lambda_Y = \Delta^{-1/2}\Lambda_X = \Delta^{-1/2}\operatorname{Cov}(X, f) = \Delta^{-1/2}\operatorname{Cov}(X, f)\underbrace{I^{-1/2}}_{\text{sd of f}}$$

TODO: CHECK

so Λ_Y is the correlation matrix between X and f, $\Lambda_Y = \operatorname{Corr}(X, f)$

If we work on original data Λ_X is the covariance matrix between the observed and the latent variables; if otherwise we work on the standardized data the Λ_Y is the correlation matrix between the observed and the latent variables.

4.5 Model identifiability

Before moving to estimation issues we need to focus a little bit on what is known as identifiability.

Definition 4.5.1. A model is said to be identifiable if a solution to the estimation problem *exists* and *it is unique*.

Let's focus of a single solution existence: actually our condition are not enough to prove that there is just one solution, there are infinity of models satisfying all the conditions above and a single factor model is not identifiable. So anyone trying to estimate a model obtain a different estimate.
Now we will prove that the solution to the estimation problem is not unique: this is because the linear factor model is invariant after orthogonal rotations. There's an infinity of factor models.
Seems a drawback but it will be useful in the future. Once we fix this problem it turns out to be a benefit.
Let's consider an orthogonal matrix called $\mathbf{G}$ such that

$$\mathbf{G}^T\mathbf{G} = \mathbf{G}\mathbf{G}^T = \mathbf{I}$$

now let's consider our model

$$\begin{aligned} X &= \Lambda f + u \overset{(1)}{=} \Lambda I f + u \\ &\overset{(2)}{=} \underbrace{\Lambda G}_{\Lambda^*}\underbrace{G^T f}_{f^*} + u \end{aligned}$$

where in (1) we inserted an I and in 2 we just replaced by GG^T. Calling ΛG as Λ^* and $G^T f$ as f^* we end up with

$$X = \Lambda^* f^* + u$$

So we can take infinite number of orthogonal matrixes and we obtain two models that has the same properties (f^* has the same property of f, and it means that

TODO: CHECK

Let's prove the two models

$$X = \Lambda f + u$$
$$X = \Lambda^* f^* + u$$

are completely equivalent. In fact start by computing expected valuees

$$\mathbb{E}\left[f^*\right] = \mathbb{E}\left[G^T f\right] = G^T \cdot \underbrace{\mathbb{E}\left[f\right]}_{=\mathbf{0}} = \mathbf{0}$$
$$\mathbb{E}\left[f^* f^{*T}\right] = \mathbb{E}\left[G^T f f^T G\right] = G^T \cdot \underbrace{\mathbb{E}\left[f f^T\right]}_{\mathbf{I}} G = G^T G = I$$

again the common factor have unit variances and are uncorrelated as the ones considered before.

Final check: what's the relationshib between f and u

$$\mathbb{E}\left[f^* u^T\right] = \mathbb{E}\left[G^T f u^T\right] = G^T \underbrace{\mathbb{E}\left[f u^T\right]}_{=\mathbf{0}} = \mathbf{0}$$

so we proved that common factor and unique factor are uncorrelated so teh two models are indistingushiable, have the same property.

Point is that We have an infinity (as the orthogonal matrixes) of equivalent solutions: so people started to try to find an unique solution.
In order to guarantee that a unique solution is obtained we need to fix something else. we impose the constraint that

$$\Lambda^T \Psi \Lambda \quad \text{is diagonal}$$

it is a constraint based on bayesian inference (basically all the software do this): Λ and Ψ cannot be whatever but must be that the quadratic form above is diagonal. By putting this constraint we obtain a single solutions.

When we'll move to interpretation is fine to have a lot of solution.

Existence We proved how to obtain a unique solution, we need to verify if it exists. As seen all what appears on right hand side of $\mathbf{X} = \mathbf{\Lambda f} + \mathbf{u}$ is unknown so there's a lot of things to be estimated.

It's not possible to estimate all in one shot: first we estimate Λ and Ψ (for $\Sigma = \Lambda\Lambda^T + \Psi$) and then we estimate f. Also this problem of estimating Λ and Ψ is a little bit tricky. The starting point of our estimation procedure

$$\Sigma = \Lambda\Lambda^T + \Psi$$

we know the elements of Σ only.
How many are the *unique* elements of Sigma, our pieces of information? It's the sum of first p natural numbers, that is $p(p+1)/2$. We want to reconstruct these elements using $p(p+1)/2$ equations and we want to find the unknows on the other side. Our unknowns are the $p \cdot m$ elements of Λ plus p diagonal elementsof Ψ.
In order to obtain of solutions the number of equations must be larger than the number of unknows;

- on the right hand side we have $p \cdot m + p$ unknowns
- we put a constraint: Λ and Ψ must satisfy $Lambda^T PsiLambda$ is diagonal matrix. This reduces the number of unknown since off diagonal elements fixed to be zero: the matrix is $m \times m$ so we have $m \cdot (m-1)/2$ element fixed/constrainted to 0

$$\begin{aligned} &\frac{p(p+1)}{2} \quad \text{equations} \\ &pm + p - \frac{m(m-1)}{2} \quad \text{unknowns} \end{aligned}$$

In order for a solution to exists

$$\frac{p(p+1)}{2} > pm + p - \frac{m(m-1)}{2} \tag{4.1}$$

p is given (number of variables we have), we need to chose m such that this equality is satisfied (so not all the value of m).
This is the condition of maximum number of common factor we can include in the model: this condition is known in literature as Ledermans condition which puts a limit on the maximum number of common factor that can be included in a factor model with p observed variable.
In order to have solution one could set $\geq$ in the ledermans inequality: the reason we put strict $>$ is that we want to have dimension reduction as well.

TODO: check

4.6 Estimation of the linear factor model

We estimate our population covariance matrix Σ using S (using either the correct or biased version), while ρ is estimated using R
The model is complicated and estimation is performed in two stages:

1. we start the estimation of the model by trying to estimate Lambda and Ψ first we try to estimate this decomposition

$$\Sigma = \Lambda\Lambda^T + \Psi$$

2. then we estimate the factor scores

Starting with the first we try to estimate the decomposition on sample quantities

$$S = \hat{\Lambda}\hat{\Lambda}^T + \hat{\Psi}$$

how to decompose S in the sum above? This estimation issue can be tackled in at least **two different ways**/approaches. We see

1. *principal factor method*: it is a distribution free method, we don't need to make any assumption on the probability density function of $\mathbf{X}$ in the population;

2. *maximum likelihood method*, that assumes normality, $\mathbf{X}$ is normally distributed

Both methods need to start from a preliminary solution and refine it until they find a good solution: so we start from a plausible estimate of the communalities. Remembering the communalities (part of observed variance accounted for by the common factors, parts of variability shared with other variables) are:

$$h_i^2 = \sum_{k=1}^{m} \lambda_{ik}^2$$

that is for each row of Λ we have the sum of its squares.

So communality of X_i is part of the variance of X_i which is explained by the common factors (shared by all the variables). As starting point for it we can adopt different strategies, which are different regarding the matrix we're working with (correlation R of standardized variables or covariance S of unstandardized variables)

1. r-squared-like: to have the part explained we can take the r_{io}^2 of X_i regressed on the *other/remaining* X's. In case of
   - R: we use it directly, that is
     $$\hat{h}_i^2 = r_{io}^2$$
   - in case of S we multiply it by the i-th variable variance to have the quantity explained
     $$\hat{h}_i^2 = s_i^2 \cdot r_{io}^2$$
2. we could use the max (absolute) correlation among X_i and any other variable $X_{i'}$ (absolute value is needed because percentage explained is positive). With
   - R: we use it directly
     $$\hat{h}_i^2 = \max_{i'} |r_{ii'}|$$
   - in case of S we again multiply it by the i-th variable variance
     $$\hat{h}_i^2 = s_i^2 \cdot \max_{i'} |r_{ii'}|$$
3. we just set to the maximum value possible. In this case we get principal component. This means that unique factors does not exists/aren't needed: common factors are able to explain variances/covariances. For
   - for R
     $$\hat{h}_i^2 = 1$$
   - for S:
     $$\hat{h}_i^2 = s_i^2$$

TODO: check

4.7 Principal factor method

Let's start from S. We build what we call the reduced covaraince matrix. At population level we have that

$$\Sigma = \Lambda\Lambda^T + \Psi$$

so i can write

$$\Sigma - \Psi = \Lambda\Lambda^T$$

what happens in the observed case, not population level

$$S = \hat{\Lambda}\hat{\Lambda}^T + \hat{\Psi} \implies S - \hat{\Psi} = \hat{\Lambda}\hat{\Lambda}^T$$

with $S - \hat{\Psi}$ called reduced covariance matrix.
The reduced covariance matrix is identical to S, but have communality on main diagonal instead of variances

$$S - \hat{\Psi} = \begin{bmatrix} \hat{h}_1^2 & s_{12} & \dots & s_{1p} \\ & \hat{h}_2^2 & \dots & s_{2p} \\ \dots & & & \\ & & & h_p^2 \end{bmatrix}$$

Reduced covaraince matrix is still squared symmetric (changed only the diagonal of a symmetric matrix) but no longer positive semidefinite (change diagonal entries). This means that no longer eigenvalue.. **TODO**: CHECK

As squared symmetric matrix can be decomposed using spectral decomposition

$$S - \hat{\Psi} = \Gamma L \Gamma^T$$

now i consider the positive eigenvalue only. I assume their number is m. So i have that

$$S - \hat{\Psi} \overset{(0)}{\approx} \Gamma_m L_m \Gamma_m^T$$
$$\overset{(1)}{=} \underbrace{\Gamma_m L_m^{1/2}}_{\Lambda} \underbrace{L_m^{1/2} \Gamma_m}_{\Lambda^T}$$

where in

- (0) L_m is the diagonal matrix of the positive eigenvalues
- (1) i substituted $L_m = L_m^{1/2} L_m^{1/2}$

So using the spectral theorem I found a way to have an estimate

$$\hat{\Lambda} = \Gamma_m L_m^{1/2}$$

If we want to obtain $\hat{\Psi}$

$$\hat{\Psi} = S - \hat{\Lambda}\hat{\Lambda}^T$$

this matrix

- is know as the residual covariance matrix
- is very important in order to check model fit: if diagonal we're happy, if not our model give poor fit to the data. If large entries are present in the off-diagonal part of $\hat{Psi}$, this means that the model gives a poor fit, as the common factors turn out to be unable to explain the observed covariances. We expected Ψ to be diagonal; if $\hat{Psi}$ elements out of main diagonal are small it's still ok

Poor performance could be dued

- take into account too few factors
- relationship between varaiable is not linear. our model is linear

Once estimated the diagonal elements of $\hat{LambdaLambda}^T$ are the final estimates for the communalities.

Scale equivariance Last comment:

- the factor model is scale equivariant
- however we're estimating factor model using spectral decomposition which is not scale equivariant, estimates obtained by the principal factor method are not scale equivariant. Thus we cannot transform estimate obtained with unstandardized variable to obtain the estimate obtained with standardized variables. As a consequence, model fitted on the raw data or on the standardized ones are different and there is no way to go from one solution to the other

Example 4.7.1 (Esempio cartaceo scores)**.** In the sheet there are some pretty high correlation: pupils with high grades on some subject tends to have high grades in other subjects.
Interpretation of the factor loading matrix: We have two latent variables

1. The first factor is more or less equal important in all the variables: this factor people say is a general value of general intelligence (if high, being positively correlated, one performs well everywhere) while low value of this tend to perform poorly. This is generally considered as general intelligence factor
2. the second factor: large values on this factor has very good score on animal house to block design, but one is very bad in math comprehension. This is math/linguistic vs art/picture tendency.
   Furthermore some variables are not relevant here such as geometric design (coefficient close to 0)

Last column is interesting: once fitted the model we can obtain final estimates for the commualities: that is

$$\hat{h}_1^2 = \lambda_{11}^2 + \lambda_{12}^2$$
$$0.713 = 0.776^2 + (-0.333)^2$$

How good is my model in reproducing the observed correlation? in general we have that

$$\sigma_{ii'} = \sum_{k=1}^{n} \lambda_{ik}\lambda_{i'k}$$

we want to study the correlation between information and vocabulary which is $\operatorname{Corr}(Information, vocabulary) = 0.755$ (the true correlation in the table) how good is my model to reconstruct the observed 0.755? The reconstructed correlation is

$$\operatorname{Corr}(Information, \hat{Vocabulary}) = 0.776 \cdot 0.823 + 0.333 \cdot 0.224 = 0.71324$$

So if i take the difference of the two

$$0.755 - 0.71324 = 0.04176$$

This final one is the entry in the residual correlation of information and vocabulary: given a matrix with all these residual I can study it to know how well my model fit the data.
In the second page of the sheets the matrix are those residual values (not exactly the same because estimated using ML, while we used principal factors method above). All the elemnts are very close to 0; the model gives a pretty good fit to the data.

Important remark 33. last point: consider the definition we've given on the communality

$$h_i^2 = \sum_{k=1}^{m} \lambda_{ik}^2$$

which is the part of variance of X_i which is explained by the m common factor. If we split this sum and focus on the single terms of the sums

$$h_i^2 = \lambda_{i1}^2 + \lambda_{i2}^2 + \ldots + \lambda_{im}^2$$

we have that λ_{i1}^2 is the part of variance of $X_i$which is explained by the first common factor. In this case for information the part is 0.776^2; for the second variable it's 0.823^2.
If I consider the trace of covariance matrix I have the total variance.

$$\operatorname{Tr} S = \text{Total variance}$$

while in case of standardized variables the total variance is equal to the number of variables ($\operatorname{Tr} R = p$).
If I sum with respect to all the variables

$$\sum_{i=1}^{p} \frac{\lambda_{i1}^2}{p}$$

i obtain the *part of total variance explained by factor 1.* So I have an idea of how a factor explain

Important remark 34 (Recappino). We're interesting in fitting $X = \Lambda f + u$: this is a linear model we're interested in, which is aimed at explaining covariances (or correlations)
However there are too many parameters (all right hand side is unknown).
Under some assumptions we're able to decompose, if the model holds, Σ as

$$Sigma = LambdaLambda^T + Psi$$

where Λ is the factor loading matrix, but also it is the covariance matrix between the observed variables and the common factors (if we deal with std variable will be also the correlation matrix between obs value and common factors).
In order to estimate this decomposition $\Sigma = \Lambda\Lambda^T + \Psi$ we estimate Σ with S, then we obtain a preliminary estimate for the communalities, which are the diagonal entries of Σ

$$sigma_i^2 = h_i^2 + psi_{ii}$$

obtaining the reduced covariance matrix $(S - \hat{\Psi})$.
There are two methods to estimate the model:

TODO: checkhere

1. principal factor methods: based on the spectral decomposition of S - hatPsi (which is the reduced covariance matrix, S with diagonal entries replaced with the preliminary communalities). Thus we obtain factor loading matrix etc etc.
   Then we've seen an example; analysis performed on CORRELATION MATRIX. the first factor is positively correlated with all variable (eg a large value will have higher grades in all the subject, so we can think it as a measure of general intelligence. The second factor is a contrast: negative correlated with first block and positively with last: a large score with this will lgave high grade with last variables and low grade with the first. can be interpred as.
   The second part of table gives info on communalities: initial guesses are R^2_{io}, were interested in the last column that is the final values of communality. If we were working on the raw data we needed variances. In general

   TODO: check

   $$\sigma_i^2 = \sum_{k=1}^{m} \lambda_{ik}^2 + \psi_{ii}$$

   but with standardized data we have that $\sigma_i^2 = 1$. otherwise it's s_i^2 so we need to know this in advance $(S' = \hat{\Lambda}\hat{\Lambda}^T + \hat{\Psi})$ Out of diagonal entries we have

   $$\sigma_{ii'} = \sum_{k=1}^{m} \lambda_{ik}\lambda_{i'k}$$

   with standardized data $\sigma_{ii'}$ is a correlation.
   Using the example, the correlation between X_1 and X_2 explained by the common factor is

   $$\hat{r}_{12} = 0.716 \cdot 0.823 + (-0.333) \cdot (-0.224)$$

we hope that $\hat{r}_{12}$ is near to r_{12} observed (0.755). The only difference here is thatwe obtain the residual correlation matrix (such as that in the higher part of page 493 of the example)

We've said that λ_{11}^2 is the part of the variance of X_1 accounted for by f_1, while λ_{12}^2 is the part of variance of X_1 accounted/explained by f_2 and $\hat{h_i}^2 = \lambda_{11}^2 + \lambda_{12}^2$ is the part of the variance of X_1 which is explained by the common factors.
As we're dealing with std vars in this example, the variance of $X_1 = 1$
Now $\hat{lambda}_{21}^2$ is the part of the variance of X_2 accounted for by factor 1 and again the variance of X_2 is 1.
now $\hat{\lambda}_{p1}^2$ is the part of the variance of X_p accounted for by factor 1 and again the variance of X_p is 1.
The trace $\operatorname{Tr} R = p$ is the total variance (number of variables) (if we were dealing with non std variables the total variance would be tr(S)).
if i take the sum

$$\frac{\sum_{i=1}^{p} \hat{\lambda_{i1}^2}}{p} \cdot 100$$

this is the percentage of the total variance which is explained by the first factor f_1. In the sheets that percentage is 48%: the first factor is able to explain the 48% of total valriability.

4.8 ML method

Second method we see for estimation is Maximum Likelihood. When Spearman invented this model, the only estimation available was the previous one (ML was not available, while spectral decomposition was). Then people started saying; i would prefer to have a way to formally test if say two factor are enough; when ML was introduced people reset the problem above with ML.

We need to specify the distribution in the population: tipically we assume that X is MVN with parameters μ, Σ

$$X \sim \text{MVN}\left(\boldsymbol{\mu}, \boldsymbol{\Sigma}\right)$$

the pdf of MVS is

$$f(\mathbf{x}) = \det 2\pi\boldsymbol{\Sigma}^{-1/2} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

within the exponential we have the mahalanobis distance between a unit and the mean of the distribution.
the likelihood will be (assuming independence of observations

$$L(x;\boldsymbol{\mu},\boldsymbol{\Sigma}) = \prod_{i=1}^{n} f(x) = \det 2\pi\Sigma^{-n/2} \exp\left\{-\frac{1}{2}\sum_{j=1}^{n}(\mathbf{x}_j-\mu)^{\mathbf{T}}\boldsymbol{\Sigma}^{\mathbf{-1}}(\mathbf{x_j}-\mu)\right\}$$

the logarithm allows us to get rid of exponential part

$$l(x;\mu,\Sigma) = -\frac{n}{2}\log\det 2\pi\Sigma - \frac{1}{2}\left\{\sum_{j=1}^{n}(\mathbf{x}_j-\mu)^{\mathbf{T}}\boldsymbol{\Sigma}^{\mathbf{-1}}(\mathbf{x_j}-\mu)\right\}$$

what happens is that we can rewrite this quantity as

$$l(x;\mu\Sigma) = -\frac{n}{2}\log\det 2\pi\Sigma - \frac{1}{2}\operatorname{Tr}\Sigma^{-1}S - \frac{n}{2}(\overline{x}-\mu)^T\Sigma^{-1}(\overline{x}-\mu)$$

The ML estimate for mean $\boldsymbol{\mu}$ is sample mean $\bar{\mathbf{x}}$ if we substitute $\overline{x}$ to μ then the quadratics in the third term disappears and we have that

TODO: check non chiarissimo nei miei appunti se ho copiato bene

$$l(x;\mu\Sigma) = -\frac{n}{2}\log\det 2\pi\Sigma - \frac{n}{2}\operatorname{Tr}\Sigma^{-1}S$$

If $\Sigma = \Lambda\Lambda^T + \Psi$ holds, then

$$l(x;\Sigma) = l(x;\Lambda,\Psi) = -\frac{n}{2}\log\det 2\pi(\Lambda\Lambda^T+\Psi) - \frac{n}{2}\operatorname{Tr}(\Lambda\Lambda^T+\Psi)^{-1}S$$

Deriving with respect to Λ and Ψ and set the derivatives $= 0$, unfortunately this equation dont admit a close formed solution: there's no formula to compute Λ and Ψ directly. It took up to the 70's: Joreskoe provided a numeric algorithm to solve the problem, so numeric methods are used to obtain numeeric estimates for Λ and Ψ.

Example 4.8.1. back to the sheet example the estimates using ML are close but not the same

Scale equivariance

One important aspecct is that ML estimates are *scale invariant*: if we fit the factor model with ML on std data, we can go back to factor model on original variables by applying the same scale change.

Differently from previous method (spectral decomposition) both *method* and *estimates* are scale equivariant.
maximum likelihood yields scale equivariant estimates: this means that after fitting the model to the raw data we can obtain the ones referred to the standardized data by simply rescaling them.
Lambda is the covariance matrix the observed variables and the common factors. Let call it $\hat{\Lambda}_X$. If i am interested in $\hat{Lambda}_Z$ (referred to the standardized variables) i simply need

TODO: check

$$\hat{\Lambda}_Z = D^{-1/2}\hat{\Lambda}_X I_m^{-1/2} = D^{-1/2}\hat{\Lambda}_X$$

Λ is a covariance, to obtain a correlation I have to divide by std deviation (at left we have std of X, at right the std of common factor which is standardized).

This transformation can be done only with ML estimates because scale equivariant.

Hypothesis testing

The fact that we're using ML allows us to perform hypothesis testing on number of factors to take: before the decision was based on residual covariance matrix. Wow under normality assumtpion we can test if a given number of factors is enough. we test sequentially: we start with a model with 1 factor. the test is

$$H_0 : sigma...$$
$$H_1 : \text{is unstructured (different from model in } H_0)$$

the test statistics is the W statistics in the example (this is the LRT statistic). As all LRT is distributed asympotetically as Chisq with df which depend on n of variable and factors (p is fixed, m is change via via).
We start testing the hypothesis with 1 factor: is 1 factor enough? we estimate all the components in W if we refuse the null we need to increment by 1 the number of factors

1. At first step we have 0.007: we decide to reject null (that 1 factor is enough) and need to increment number of factors
2. we fit a two factor model: p-value is 0.92 so we don't reject the null and the model is ok to take two factor

TODO: CHECK ultima considerazione

we're seeking linear factor: if we reject the model with maximum number of factor there's some problem with the model, not the number of factors

4.9 Factor rotation

H in the sheet is an orthogonal matrix

if we compute $Lam\hat{b}daH$ (orthogonal rotation) we obtain a new solution in Γ^*

the new model has the same properties of the original one

It was G in the notes the orthogonal matrix wi

One way to check that the solution is the same is to compute the communalities: if one do the computations, we obtain the same communality for the first variable.

Same holds for the explained covariances.

this is what invariance after orthogonalrotation means.

Why are we interested in rotations? Thurstone (psychometrician) in 1947 wrote a paper which defined what a *simple factor structure* is.

Definition 4.9.1. If the factor strucuture is simple, the variables should be divisible into gorups such that hte loadings, within each group, are high on a single factor, perhaps moderate to low on a few factors and negligible on the remaining factor.

Eg if we have three common factor with these loadings (H = high, M = moderate, 0 = null)

$$\Lambda = \begin{bmatrix} H & M & 0 \\ H & M & 0 \\ H & M & 0 \\ 0 & H & M \\ 0 & H & M \\ M & O & H \\ M & O & H \end{bmatrix}$$

Interpreting here is easier. this is tipically not the case with unrotated factors where the first is a general (and other are contrasts).

There are a lot of rotations: most widely known are

- varimax (orthogonal, uncorrelated factors)
- quartimax (orthogonal, uncorrelated factors)
- oblimin (not orthogonal, correlated)

The first twos maximizes something, the last minimize something. In the last obli means *oblique* rotations so it provides correlated factors)

4.9.1 Variamax

An idea of how VARIMAX works. We maximize a function V

$$V = \sum_{k=1}^{m} \left[\overbrace{\underbrace{\frac{\sum_{i=1}^{p} \beta_{ik}^4}{p}}_{(A)} - \underbrace{\left(\frac{\sum_{i=1}^{p} \beta_{ik}^2}{p} \right)^2}_{B}}^{C} \right]$$

where

$$\beta_{ik} = \frac{\lambda}{\sqrt{\sum_{k=1}^{m} \lambda_{ik}^2}} = \frac{\lambda_{ik}}{h_i}$$

Starting from β_{ik}: numerator is usual loading of variable i on factor k. Denominator is sum of squared loadings in the row with sqrt (sqrt of communality), it's the norm of the row vector

So the ratio is a kind of normalization of λ_{ik} by the norm so the matrix which is obtained in this way has row that has unit norm . **TODO**: CHECK

Now going to the main equation:

- summation works inside the columns of the obtained normalized matrix: within parenthesis there's a sort of variance
- both each components inside square brackets are shit column wise: at the numerator we have the fast variance formula, inside squared brackets i have variance of squared beta values in column k

so in essence looking at the main equation of V:

- (A) is the square of quadratic mean of β
- (B) is the arithmetic mean of squared β (kind of variance)
- C is variance of β values in column k.

Point is: **we maximize the sum of the variances inside of each column**. We obtaine large weights on some factor and low weights on other one.

If the original solution obtained is difficult to interpret, we can apply this transformation to ease/optimize it.

4.10 Factor score estimation

Remembering our factor model was

$$X = \Lambda f + u$$

now we are able to estimate Λ by $\hat{\Lambda}$ (using ML or the other).
We **want now to estimate** f, in order to end with an estimate of $\mathbf{u}$.

I can say that for factor k, the score for factor k is obtainable as linear combination of value of $\mathbf{x}$: i can measure how good is f_k^* in predicting f_k.

4.10.1 Thompson

I want to find f_k^* such as :

$$\mathbb{E}\left[(f_k^* - f_k)^2\right] \quad \text{is the smallest}$$

This quanity is a funciton of a_k

$$\phi = \mathbb{E}\left[(a_k^T x - f_k)^2\right]$$

we want to find a_k for which ϕ is minimum; so go with derivatives and set $= 0$

$$\frac{\partial \phi}{\partial a_k} = \mathbb{E}\left[2x(x^T a_k - f_k)\right] = 2\,\mathbb{E}\left[xx^T\right] a_k - 2\,\mathbb{E}\left[x f_x\right]$$

where $\mathbb{E}\left[xx^T\right]$ is cov matrix of X and with mean centered data $\mathbb{E}\left[x f_x\right]$ is variance/covaraince between X and f_x thus the k-th column of Λ (call it Λ_k) so we have

$$\frac{\partial \phi}{\partial a_k} = 2\Sigma a_k - 2\Lambda_k = 2(\Sigma a_k - \Lambda_k)$$

by putting $2(\Sigma a_k - \Lambda_k) = 0$ and solving for a_k we obtain

$$a_k = \Sigma^{-1}\Lambda_k$$

So

$$f_k^* = a_k^T x = \Lambda_k^T \Sigma^{-1} x$$

then making this for all the factor $k = 1, \ldots, m$ and collect in matrix i have

$$F^* = \Lambda^T \Sigma^{-1} x$$

it can be proved that F^* can equivalently be written as

$$F^* = \left(\mathbf{I} + \Lambda^T \Psi^{-1} \Lambda\right)^{-1} \Lambda^T \Psi^{-1} X$$

this formula is known as *Thompson estimator* (estimator for factor scores).

Properties of estimator What are the property of this estimator?

- minimize the squared prediction error (by definition/derivation): it has been obtained by minimizing the expected squared prediction error. But if we compute the expected value

$$\begin{aligned}\mathbb{E}\left[F^*|F\right] &= \mathbb{E}\left[(\mathbf{I}+\Lambda^T\Psi^{-1}\Lambda)^{-1}\Lambda^T\Psi^{-1}X|F\right] \\ &= \underbrace{(I+\Lambda^T\Psi^{-1}\Lambda)^{-1}\Lambda^T\Psi^{-1}}_{\text{all constants}}\cdot\mathbb{E}\left[X|F\right]\end{aligned}$$

  but considering $X = \Lambda f + u$

$$\mathbb{E}\left[X|F\right] = \mathbb{E}\left[\Lambda f + u\right] = \Lambda f + \underbrace{\mathbb{E}\left[u\right]}_{=0} = \Lambda f$$

  with Λf constant since conditioning. So coming back we have that

$$\mathbb{E}\left[F^*|F\right] = \underbrace{(I+\Lambda^T\Psi^{-1}\Lambda)^{-1}\Lambda^T\Psi^{-1}\Lambda}_{\neq I} F \neq F$$

  So $EF^*|F \neq F$ and this estimator is biased

TODO: buono in termini di prediction error? controllare registrazioni

4.10.2 Bartlett estimator

Another solution for estimating F resorting to Bartlett's estimator. Our model is still $X = \Lambda f + u$ (here f a vector for a single variable) and $\text{Var}\left[u\right] = \Psi$.
If estimate Λ using $\hat{\Lambda}$ this looks like a linear regression model with uncorrelated but heteroscedastic (different variance) error; in regression residuals were expected to be omoschedastic ($\text{Var}\left[epsilon\right] = \sigma^2 I$).
Here they're not homoscedastic: with non omoschedasticity we can estimate it use *weighted least square* (weight: residual with large variance have lower weight) the function we want to minimize is

$$u^T\Psi^{-1}u = (x-\Lambda f)^T\Psi^{-1}(X-\Lambda f)$$

derive with respect fo f and set the derivatives $= 0$

$$\frac{\partial}{\partial f} = -2\Lambda^T\Psi^{-1}(X-\Lambda f) = -2\Lambda^T\Psi^{-1}X + 2\Lambda^T\Psi^{-1}\Lambda f$$

Setting the last $= 0$ we have

$$\Lambda^T\Psi^{-1}\Lambda f = \Lambda^T\Psi^{-1}X$$

in order to obtain f we need to calculate the inverse of $\Lambda^T\Psi^{-1}\Lambda$. So the estimator of bartlett is

$$\hat{f} = (\Lambda^T\Psi^{-1}\Lambda)^{-1}\Lambda^T\Psi^{-1}X$$

Properties we have that

$$\begin{aligned}\mathbb{E}\left[\hat{f}|f\right] &= \mathbb{E}\left[(\Lambda^T\Psi^{-1}\Lambda)^{-1}\Lambda^T\Psi^{-1}X|f\right] \\ &= (\Lambda^T\Psi^{-1}\Lambda)^{-1}\Lambda^T\Psi^{-1}\cdot\underbrace{\mathbb{E}\left[X|f\right]}_{\Lambda f} \\ &= (\Lambda^T\Psi^{-1}\Lambda)^{-1}\Lambda^T\Psi^{-1}Lambdaf \\ &= If = f\end{aligned}$$

so we have that it is unbiased estimator, but compared to the previous has larger varaince: previous has the lowest variance but has bias.

4.11 Relationship between PCA and Factor Analysis

One option we have when setting preliminary guess of communality is to set $=$ 1 (with standardized data) or observed variance (if working with raw data).

the Principal factor method worked on reduced covariance matrix

$$S-\hat{\Psi}=\begin{bmatrix}h_1^2 & s_{12} & \dots & \dots \\ & h_2^2 & \dots & \\ & & & h_p^2\end{bmatrix}$$

If we decide that preliminary communalities (on the diagonal) are the observed variance (in diagonal) the reduced covariance matrix is just S, just the variance covariance matrix.
The same happens if we set it to 1 when working with std data, we obtain the original correlation matrix

so in this cases the reduced covariance correlation matrix is equal to the original covariance/correlation matrix)

Principal factor method perform spectral decomposition of the reduced covariance matrix, now since this coincides with original covariance correlation it's just a PCA.

As according to our choice for the communialities $S-\hat{\Psi}$ and S coincide, extracting the factor using principal factor method amounts to perform the spectral decomposition of S, that is to obtain PCs

So setting communality $=$ 1and principal factor method we obtain PCA.

BUT assume we have X which is $p\times 1$ and the principal components $y = A^Tx$ with A has eigenvector in column.
Since A is orthogonal it inverted coincides with transpose, by premultipluing A^T with its invert

$$X = Ay$$

i split matrix **A** into two parts

$$A=\begin{bmatrix}\mathbf{A}_m & \mathbf{A}_{p-m}\end{bmatrix}$$

with A_m the first m eigenvector and $\mathbf{A}_{p-m}$ the remaining ones. Y can be splitted vertically

$$Y = \begin{bmatrix} Y_m \\ Y_{p-m} \end{bmatrix}$$

this means that X can be written as

$$X = Ay = \begin{bmatrix} \mathbf{A}_m & \mathbf{A}_{p-m} \end{bmatrix} \begin{bmatrix} Y_m \\ Y_{p-m} \end{bmatrix} = A_m Y_m + A_{p-m} Y_{p-m}$$

i can also put I in the right place and decompose it as $L_m^{1/2} L_m^{-1/2}$ (with L_m a diagonal matrix with the first m eigenvalue)

$$\begin{aligned} X &= A_m I_m Y_m + A_{p-m} Y_{p-m} \\ &= A_m L_m^{1/2} L_m^{-1/2} Y_m + A_{p-m} Y_{p-m} \end{aligned}$$

In so doing I separated first m principal compoenents on one side and the remaining on the other size. Now let's call

$$\begin{aligned} &A_m L_m^{1/2} = \Lambda \\ &L_m^{-1/2} Y_m = f \\ &A_{p-m} Y_{p-m} = \eta \end{aligned}$$

So we have that the above can be rewritten as

$$X = \Lambda f + \eta$$

Is this a linear factor model? if the answer is yes PCA is a special case of factor analysis, otherwise they are two different things. The answer is that **this is not a linear factor model**.
To check it we check whether latent variables involved in the model satisfy all the assumption; especially we want to check the linear assumptions we made

1. is true that $\mathbb{E}\left[()\, f\right) = \mathbf{0}$? we have that

   $$\mathbb{E}\left[L_m^{-1/2} Y_m\right] = \mathbf{0}$$

   because we're working with mean centered data. So this first condition is satisfied

2. is common factor uncorrelated and have unit variance, that is $\mathbb{E}\left[ff^T\right] = \mathbf{I}$? we have

   $$\mathbb{E}\left[ff^T\right] = \mathbb{E}\left[L_m^{-1/2} Y_m Y_m^T L_m^{-1/2}\right] \overset{(=)}{1} L_m^{-1/2}\, \mathbb{E}\left[Y_m Y_m^T\right] L_m^{-1/2}$$

   whhere in (1) we take $L_m^{-1/2}$ out of expectation. WHat is $\mathbb{E}\left[Y_m Y_m^T\right]$? It's the variance/covariance of the first m principal components, a diagonal matrix with eigenvalues on diagonal, L_m. So we have

   $$\mathbb{E}\left[ff^T\right] = L_m^{-1/2} L_m L_m^{-1/2} = L_m^{-1/2} L_m^{1/2} L_m^{1/2} L_m^{-1/2} = \mathbf{II} = \mathbf{I}$$

   so ok, the property is verified

3. is $\mathbb{E}\left[eta\right] = \mathbf{0}$? We have

$$\mathbb{E}\left[\eta\right] = \mathbb{E}\left[A_{p-m} Y_{p-m}\right] = A_{p-m}\,\mathbb{E}\left[Y_{p-m}\right] \overset{(1)}{=} \mathbf{0}$$

   where in (1) we have that $\mathbb{E}\left[Y_{p-m}\right] = \mathbf{0}$ because mean centered.
   So even this this is satisfied

4. property foundamental which relates common factor and unique factors, that is $\mathbb{E}\left[f^T eta\right] = \mathbf{0}$

TODO: non chiarissima la trasposizione qui check

$$\mathbb{E}\left[f^T \eta\right] = \mathbb{E}\left[f \eta^T\right] = \mathbb{E}\left[L_m^{-1/2} Y_m Y_{p-m}^T A_{p-m}^T\right] = L_m^{-1/2}\,\mathbb{E}\left[Y_m Y_{p-m}^T\right] A_{p-m}^T$$

   where $\mathbb{E}\left[Y_m Y_{p-m}^T\right]$is the covariance between the first m components and the last p-m ones. This is $\mathbf{0}$ because pcs are uncorrelated so actually all is 0 and check is verified

5. is $\mathbb{E}\left[\eta\eta^T\right]$ a diagonal matrix? remembering

$$\Psi = \begin{bmatrix} \psi_{11} & 0 & 0 \\ 0 & \psi_{ii} & 0 \\ 0 & & \psi_{pp} \end{bmatrix}$$

   is $\mathbb{E}\left[\eta\eta^T\right]$ similar to this one? we have

$$\mathbb{E}\left[\eta\eta^T\right] = \mathbb{E}\left[A_{p-m} Y_{p-m} Y_{p-m}^T A_{p-m}^T\right] = A_{p-m}\,\mathbb{E}\left[Y_{p-m} Y_{p-m}^T\right] A_{p-m}^T$$

   where $\mathbb{E}\left[Y_{p-m} Y_{p-m}^T\right]$is the variance covariamce of last $p-m$ components, it's a diagonal matrix with last $p-m$ eigenvalues (it's L_{p-m}). It is a diagonal matrix but if the entries/diagonal elements are different this is not enough: in general diagonal elements are different so the whole product is not diagonal, that is $\mathbb{E}\left[\eta\eta^T\right]$ is not diagonal.
   The condition does not hold: the unique factor η are not uncorrelated, and this means that in the model

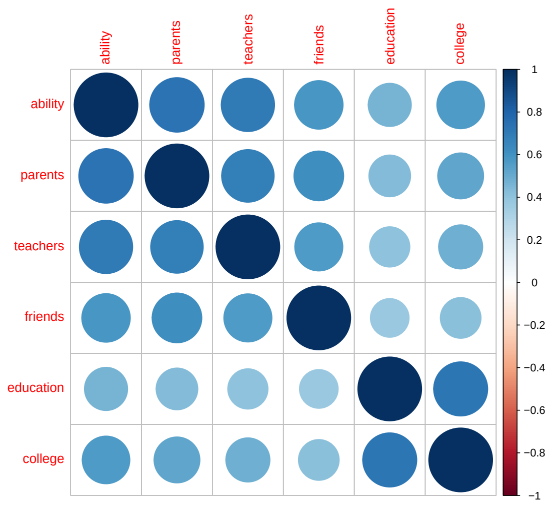
$$X = \Lambda f + \eta$$

   the commond factors f are not able to explain the observed covariances (which was the goal of fitting a factor model)

Important remark 35. If we decide to put communality = 1 or observed variances the algo fits principal components, but this is not a model: its just PCA because it does not satisfy all the requirements of FA.
People wrongly think that what can be done in FA can be done in PCA (eg rotating); this is just wrong. the property of Linear factor model does not holds with PCA

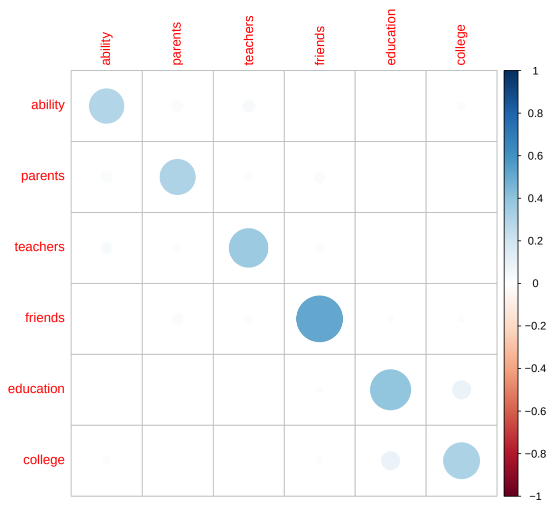
4.12 Lab

```
ability <- read.table("data/ability-education.txt")
## in this case this is a correlation matrix between variables

## need to transform it in a matrix
(R <- as.matrix(ability))

##           ability parents teachers friends education college
## ability      1.00    0.73     0.70    0.58      0.46    0.56
## parents      0.73    1.00     0.68    0.61      0.43    0.52
## teachers     0.70    0.68     1.00    0.57      0.40    0.48
## friends      0.58    0.61     0.57    1.00      0.37    0.41
## education    0.46    0.43     0.40    0.37      1.00    0.72
## college      0.56    0.52     0.48    0.41      0.72    1.00

# we have quite high correlation all positive, it makes sense to perform factor
# analyusis
## with higher number of variable visualizzation plot is useful
library(corrplot)

## corrplot 0.95 loaded

corrplot(R)
```



```
## 1) principal factor method by hand
## first thing to do is to have a preliminary value of communality: we use
## the multiple correlation coefficient 1-1/r_ii* with i-th diagonal element of
## R^_{-1}

(h2tilde <- 1 - 1/diag(solve(R))) # diagonal of the inverse of correlation matrix

##   ability   parents  teachers   friends education   college
## 0.6427569 0.6248924 0.5695938 0.4358076 0.5265227 0.5928205
## at denominator

# these are the preliminary estimates of communalities
## we compute the reduced correlation matrix

redR <- R # replace diag with preliminary estimates of comm
diag(redR) <- h2tilde
redR # no more 1 on diagonal

##              ability   parents  teachers   friends education   college
## ability   0.6427569 0.7300000 0.7000000 0.5800000 0.4600000 0.5600000
## parents   0.7300000 0.6248924 0.6800000 0.6100000 0.4300000 0.5200000
## teachers  0.7000000 0.6800000 0.5695938 0.5700000 0.4000000 0.4800000
## friends   0.5800000 0.6100000 0.5700000 0.4358076 0.3700000 0.4100000
## education 0.4600000 0.4300000 0.4000000 0.3700000 0.5265227 0.7200000
## college   0.5600000 0.5200000 0.4800000 0.4100000 0.7200000 0.5928205

## to compute factor loadings: we need to compute low rank approximation (check)

## to do SVD
spectral <- eigen(redR)
spectral$values # eigenvalues: only first two are positive. this because

## [1]  3.33126929  0.47350875 -0.04368765 -0.08468263 -0.11304912 -0.17096486

# reduced is not positive definite. looking at eigen we can think considering
# that two factor should be enough, m should be 2

## we build the matrix of eigenvector with just 2 eigenvectors and vectors of
## eigenvalue with just 2 eigenvalues,

## then we construnt
## lambda = gamma_m L_m^{1/2} # looking at the used

G <- spectral$vectors[, 1:2]     # gamma only hte first two columns/eigvenvector
L <- diag(spectral$values[1:2]) # diag matrix with first two eigenvalues

G %*% L %*% t(G)  # low rank approximation of correlation matrix

##           [,1]      [,2]      [,3]      [,4]      [,5]      [,6]
## [1,] 0.7072292 0.7001694 0.6668653 0.5834546 0.4685601 0.5441205
## [2,] 0.7001694 0.6955646 0.6634608 0.5801711 0.4374113 0.5137057
## [3,] 0.6668653 0.6634608 0.6332413 0.5536204 0.4057116 0.4789896
## [4,] 0.5834546 0.5801711 0.5536204 0.4840494 0.3583494 0.4222716
## [5,] 0.4685601 0.4374113 0.4057116 0.3583494 0.6043086 0.6378458
## [6,] 0.5441205 0.5137057 0.4789896 0.4222716 0.6378458 0.6803849

Lambda <- G %*% L^0.5 # factor loadings: G_m L^{1/2}
# a matrix of dimension 6x2 is what we want 2 factor 2 column, 6 variables in
# row. interpret later
```

```
## Now we compute the new communality: communality is part of variance
## explained by common factor. To extract communality,
## Lambda t(Lambda) and extract diagonal (interested only in the varainces not covariances)

(communalities <- diag(Lambda %*% t(Lambda)))

## [1] 0.7072292 0.6955646 0.6332413 0.4840494 0.6043086 0.6803849

## each values is the proportion of variability explained by the two factors
## eg 70% of ability is explained from the two factor

## extract uniqueness: diag of correlation matrix - communality
uniqueness <- diag(R)- communalities # == 1 - communalities

## CHECK THE GOODNESS OF FIT: compute residual correlation matrix (diff between
## observed and Lambda t(Lambda))
R - Lambda %*% t(Lambda) # out of main diagonal should be close to zero

##                 ability      parents     teachers      friends    education
## ability    0.292770802  0.029830608  0.033134677 -0.003454555 -0.008560141
## parents    0.029830608  0.304435440  0.016539177  0.029828913 -0.007411273
## teachers   0.033134677  0.016539177  0.366758716  0.016379562 -0.005711590
## friends   -0.003454555  0.029828913  0.016379562  0.515950562  0.011650634
## education -0.008560141 -0.007411273 -0.005711590  0.011650634  0.395691356
## college    0.015879548  0.006294259  0.001010408 -0.012271579  0.082154195
##                 college
## ability    0.015879548
## parents    0.006294259
## teachers   0.001010408
## friends   -0.012271579
## education  0.082154195
## college    0.319615088

## test mio
corrplot(R - Lambda %*% t(Lambda))
```



```
## out of diagonal low values

## TOTAL variability explained by each factor, total variability is p. To do
## that is the tr(Lambda) Lambda (Lambda il 6x2 but we want a 2x2: consider the
## transpose of Lamnda)

diag(t(Lambda) %*% Lambda) # interested in diagonal, the variance

## [1] 3.3312693 0.4735087

## so the first factor explain 3.33 and second 0.47

## percentage explained
diag(t(Lambda) %*% Lambda) / 6 # number of variables

## [1] 0.55521155 0.07891812

## first factor explain 55% of total variability, 7% for the second


## finally, to compute communality an equivalent way
apply(Lambda, 1, function(x) sum(x^2)) # same result as before

## [1] 0.7072292 0.6955646 0.6332413 0.4840494 0.6043086 0.6803849
```

```
# how to do in R. fa and factanal functions

library(psych) # psych::fa  gives both principal factor method and ML

##
## Caricamento pacchetto:  'psych'
## Il seguente oggetto è mascherato da 'package:car':
##
##     logit
## Il seguente oggetto è mascherato da 'package:lbmisc':
##
##     table2df
```

```
## vohabolario vernaholo giorentino

# n.obs is needed for p-values, we're not using it
# rotate, gives rotation to be considered
# fm: method used for estimation. default seen minres has not be seen in class,
## "pa" principal factor,
## "ml" for maximum likelihoo

pafa1 <- fa(R,
            nfactors = 2, # nfactors wanted (we already seen two positive eigenv)
            rotate = "none", # for the moment we dont' rotatae
            fm = "pa" # principal factor solution as done before
            )

pafa1

## Factor Analysis using method =  pa
## Call: fa(r = R, nfactors = 2, rotate = "none", fm = "pa")
## Standardized loadings (pattern matrix) based upon correlation matrix
##            PA1   PA2   h2   u2 com
## ability   0.83 -0.18 0.73 0.27 1.1
## parents   0.82 -0.24 0.73 0.27 1.2
## teachers  0.77 -0.24 0.66 0.34 1.2
## friends   0.67 -0.19 0.49 0.51 1.2
## education 0.67  0.48 0.68 0.32 1.8
## college   0.76  0.45 0.77 0.23 1.6
##
##                        PA1  PA2
## SS loadings           3.44 0.61
## Proportion Var        0.57 0.10
## Cumulative Var        0.57 0.68
## Proportion Explained  0.85 0.15
## Cumulative Proportion 0.85 1.00
##
## Mean item complexity =  1.3
## Test of the hypothesis that 2 factors are sufficient.
##
## df null model =  15  with the objective function =  3.3
## df of  the model are 4  and the objective function was  0.01
##
## The root mean square of the residuals (RMSR) is  0.01
## The df corrected root mean square of the residuals is  0.02
##
```

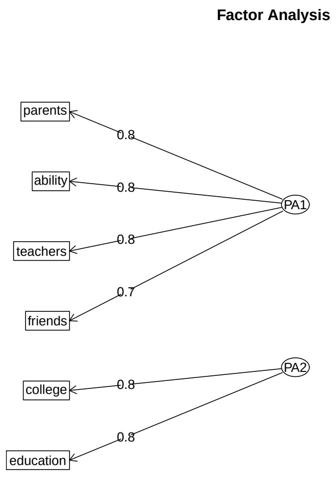
```
## Fit based upon off diagonal values = 1
## Measures of factor score adequacy
##                                                    PA1  PA2
## Correlation of (regression) scores with factors   0.96 0.83
## Multiple R square of scores with factors          0.92 0.68
## Minimum correlation of possible factor scores     0.84 0.36

pafa1$loadings # matrix of loadings

##
## Loadings:
##           PA1    PA2
## ability    0.834 -0.181
## parents    0.822 -0.236
## teachers   0.775 -0.239
## friends    0.672 -0.192
## education  0.666  0.483
## college    0.757  0.445
##
##                  PA1   PA2
## SS loadings    3.440 0.614
## Proportion Var 0.573 0.102
## Cumulative Var 0.573 0.676

Lambda # similar a part of the sign to what obtained before

##            [,1]       [,2]
## [1,] -0.8273744 -0.1506015
## [2,] -0.8103705 -0.1971401
## [3,] -0.7682259 -0.2075338
## [4,] -0.6732548 -0.1754348
## [5,] -0.6452398  0.4335599
## [6,] -0.7281779  0.3874814

## SS loadings are total variability explained
## second row is the proportion of variability

## to extract thecommunalities and uniquenesses
pafa1$communality # similar to what done before

##   ability   parents  teachers   friends education   college
## 0.7292947 0.7305715 0.6570953 0.4882353 0.6776897 0.7714643

pafa1$uniquenesses

##   ability   parents  teachers   friends education   college
## 0.2707053 0.2694285 0.3429047 0.5117647 0.3223103 0.2285357

# residual correlation matrix
pafa1$residual # off diagonal still values very close to 0 (good fit)
```

```
##                ability      parents      teachers      friends      education
## ability    0.270705253  0.001639509  0.0102526111 -0.015507856 -0.0084315471
## parents    0.001639509  0.269428492 -0.0127285853  0.012765292 -0.0034115950
## teachers   0.010252611 -0.012728585  0.3429047263  0.003724221 -0.0007200665
## friends   -0.015507856  0.012765292  0.0037242208  0.511764685  0.0147570912
## education -0.008431547 -0.003411595 -0.0007200665  0.014757091  0.3223103254
## college    0.008871656  0.002985356 -0.0001766904 -0.013570761  0.0002745308
##                  college
## ability    0.0088716563
## parents    0.0029853559
## teachers  -0.0001766904
## friends   -0.0135707613
## education  0.0002745308
## college    0.2285356519
```

```
## since loadings are not rotatad this can be difficult to be interpret, if we
## rotate it helps

pafa2 <- fa(R,
            nfactors = 2,
            rotate = "varimax", # unique change
            fm = "pa"
            )



pafa2
```

```
## Factor Analysis using method =  pa
## Call: fa(r = R, nfactors = 2, rotate = "varimax", fm = "pa")
## Standardized loadings (pattern matrix) based upon correlation matrix
##            PA1  PA2   h2   u2 com
## ability   0.79 0.33 0.73 0.27 1.3
## parents   0.81 0.28 0.73 0.27 1.2
## teachers  0.77 0.25 0.66 0.34 1.2
## friends   0.66 0.23 0.49 0.51 1.2
## education 0.27 0.78 0.68 0.32 1.2
## college   0.36 0.80 0.77 0.23 1.4
##
##                        PA1  PA2
## SS loadings           2.50 1.56
## Proportion Var        0.42 0.26
## Cumulative Var        0.42 0.68
## Proportion Explained  0.62 0.38
## Cumulative Proportion 0.62 1.00
##
## Mean item complexity =  1.3
## Test of the hypothesis that 2 factors are sufficient.
##
## df null model =  15  with the objective function =  3.3
## df of  the model are 4  and the objective function was  0.01
```

```
##
## The root mean square of the residuals (RMSR) is  0.01
## The df corrected root mean square of the residuals is  0.02
##
## Fit based upon off diagonal values = 1
## Measures of factor score adequacy
##                                                    PA1  PA2
## Correlation of (regression) scores with factors   0.91 0.88
## Multiple R square of scores with factors          0.83 0.77
## Minimum correlation of possible factor scores     0.66 0.54

## looking at the loadings, the first factor has high entries for first four
## variables, while the second has high loading fo the last variable
## now this is a dataset on 556 students which answered question:
## - ability: self concept ability
## - parents: perceived parental evaluation
## teachers: perceived teacher evaluation
## friend: perceived friends
## education
## college

# so high entries on first factor which is called perceived ability
# second factor is the attitude of the student towarrd education

# visualization of factor
fa.diagram(pafa2)
```



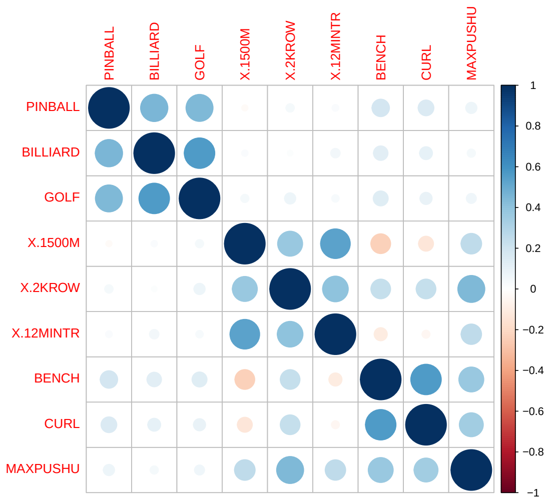
```
## PA1 first factor is highly related to the first four variables while second
## to the last two
```

```
# let's consider ML method

mlfa1 <- fa(R,
            nfactors = 2,
            rotate = "none",
            fm = "ml" # only change
            )

mlfa1

## Factor Analysis using method =  ml
## Call: fa(r = R, nfactors = 2, rotate = "none", fm = "ml")
## Standardized loadings (pattern matrix) based upon correlation matrix
##             ML1   ML2   h2    u2 com
## ability    0.57  0.64 0.73 0.266 2.0
## parents    0.54  0.66 0.73 0.274 1.9
## teachers   0.49  0.64 0.66 0.344 1.9
## friends    0.42  0.56 0.49 0.509 1.9
## education 0.72  0.07 0.53 0.471 1.0
## college    1.00 -0.02 1.00 0.005 1.0
##
##                         ML1  ML2
## SS loadings           2.56 1.57
## Proportion Var        0.43 0.26
## Cumulative Var        0.43 0.69
## Proportion Explained  0.62 0.38
## Cumulative Proportion 0.62 1.00
##
## Mean item complexity =  1.6
## Test of the hypothesis that 2 factors are sufficient.
##
## df null model =  15  with the objective function =  3.3
## df of  the model are 4  and the objective function was  0.01
##
## The root mean square of the residuals (RMSR) is  0.01
## The df corrected root mean square of the residuals is  0.02
##
## Fit based upon off diagonal values = 1
## Measures of factor score adequacy
##                                                    ML1  ML2
## Correlation of (regression) scores with factors   1.00 0.91
## Multiple R square of scores with factors          1.00 0.83
## Minimum correlation of possible factor scores     0.99 0.67

## as before
mlfa1$loadings # without rotation

##
## Loadings:
##            ML1    ML2
## ability    0.575  0.635
## parents    0.535  0.663
## teachers   0.495  0.641
## friends    0.423  0.558
## education  0.723
## college    0.997
##
##                  ML1   ML2
## SS loadings    2.558 1.571
## Proportion Var 0.426 0.262
## Cumulative Var 0.426 0.688

mlfa1$communality

##   ability   parents  teachers   friends education   college
## 0.7336711 0.7255385 0.6555405 0.4907396 0.5286846 0.9950001

mlfa1$uniquenesses

##     ability     parents    teachers     friends   education     college
## 0.266328898 0.274461521 0.344459539 0.509260352 0.471315389 0.004999905

## finally factanal: ML estimation of factor analysis
## argument are a little different:
## x is a formula or a numeric matrix (not correlation matrix, it's the data!)
## facrors: n of factors wanted
## data: data for formula in x
## covmat = covariance matrix (if we dont' have the data)
## n.obs: is needed if we want scores or chisquare p-values
## rotation: default is "varimax", if we dont' want to rotate specichiamo "none"
## scores = non (se non vogliamo gli scores), regression(thomposon)or bartlet

mlfactanal1 <- factanal(factors = 2, covmat = R, n.obs = 556, rotation = 'none')
## again
mlfactanal1$loadings  # results exactly equal to fa with ml option

##
## Loadings:
##           Factor1 Factor2
## ability    0.575   0.635
## parents    0.535   0.663
## teachers   0.495   0.641
## friends    0.423   0.558
## education  0.723
## college    0.997
##
##                Factor1 Factor2
## SS loadings      2.558   1.571
## Proportion Var   0.426   0.262
## Cumulative Var   0.426   0.688
```

```
mlfactanal1$uniquenesses

##   ability   parents  teachers   friends education   college
## 0.2663356 0.2744603 0.3444599 0.5092609 0.4713136 0.0050000

1 - mlfactanal1$uniquenesses ## communality

##   ability   parents  teachers   friends education   college
## 0.7336644 0.7255397 0.6555401 0.4907391 0.5286864 0.9950000

## interesting: since we've specified n of obs we have chisq and p-value:
## p-value is larger than usual alpha: we can conclude that two factors are
## enough to explain correlation

rm(list = ls())
```

4.13 Example with dataset instead of correlation matrix

```
## spss
library(Hmisc)

##
## Caricamento pacchetto:  'Hmisc'
## Il seguente oggetto è mascherato da 'package:psych':
##
##     describe
## Il seguente oggetto è mascherato da 'package:lbmisc':
##
##     %nin%
## I seguenti oggetti sono mascherati da 'package:base':
##
##     format.pval, units

library(foreign)

Athletics <- spss.get("data/AthleticsData.sav")
dim(Athletics) # not a square matrix, not raw data

## [1] 1000    9

## measuring scores of 1000 individuals on some sports
corrplot(cor(Athletics))
```



```
## we see two blocks of variables with quite high correlation so it make sense
## to perform factor analysis
```

```
## we consider ML method
x = Athletics
(ml2 <- factanal(x, factors = 2, rotation = "none"))

##
## Call:
## factanal(x = x, factors = 2, rotation = "none")
##
## Uniquenesses:
##   PINBALL  BILLIARD      GOLF   X.1500M   X.2KROW X.12MINTR     BENCH      CURL
##     0.938     0.962     0.955     0.361     0.534     0.536     0.301     0.540
##  MAXPUSHU
##     0.560
##
## Loadings:
##             Factor1 Factor2
## PINBALL      0.249
## BILLIARD     0.192
## GOLF         0.206
## X.1500M              0.793
## X.2KROW      0.413   0.544
## X.12MINTR            0.681
## BENCH        0.813  -0.193
## CURL         0.673
## MAXPUSHU     0.545   0.379
##
##                  Factor1 Factor2
## SS loadings        1.734   1.579
## Proportion Var   0.193   0.175
## Cumulative Var   0.193   0.368
##
## Test of the hypothesis that 2 factors are sufficient.
## The chi square statistic is 652.4 on 19 degrees of freedom.
## The p-value is 4.3e-126

## DIFFERENTLY here if we look at chisquare it's very high and p-value very
## low: we reject H_0 that our variables chan be explained by two factors.
## increase by 1 and see what happens
(ml3 <- factanal(x, factors = 3, rotation = "none"))

##
## Call:
## factanal(x = x, factors = 3, rotation = "none")
##
## Uniquenesses:
##   PINBALL  BILLIARD      GOLF   X.1500M   X.2KROW X.12MINTR     BENCH      CURL
##     0.635     0.414     0.455     0.361     0.520     0.538     0.302     0.536
##  MAXPUSHU
##     0.540
##
## Loadings:
##           Factor1 Factor2 Factor3
## PINBALL    0.425           0.429
## BILLIARD   0.443           0.624
## GOLF       0.447           0.585
## X.1500M            0.799
## X.2KROW    0.408   0.496  -0.260
## X.12MINTR          0.672
## BENCH      0.729  -0.280  -0.297
## CURL       0.605  -0.158  -0.270
## MAXPUSHU   0.512   0.317  -0.312
##
##                Factor1 Factor2 Factor3
## SS loadings      1.912   1.545   1.243
## Proportion Var   0.212   0.172   0.138
## Cumulative Var   0.212   0.384   0.522
##
## Test of the hypothesis that 3 factors are sufficient.
## The chi square statistic is 12.94 on 12 degrees of freedom.
## The p-value is 0.373

# ok p.value is larger and we don't reject h0 so 3 latent variables are ok for
# this dataset

## looking at the plot it seemed that two were enough, but loking better there
## are 3 blocks. corrplot is just a visual plot

ml3$uniquenesses
```

```
##   PINBALL  BILLIARD      GOLF   X.1500M   X.2KROW X.12MINTR     BENCH      CURL
## 0.6350926 0.4136649 0.4554615 0.3611385 0.5195340 0.5378475 0.3019471 0.5358651
##  MAXPUSHU
## 0.5396343
```

```
ml3$loadings
```

```
##
## Loadings:
##           Factor1 Factor2 Factor3
## PINBALL    0.425           0.429
## BILLIARD   0.443           0.624
## GOLF       0.447           0.585
## X.1500M            0.799
## X.2KROW    0.408   0.496  -0.260
## X.12MINTR          0.672
## BENCH      0.729  -0.280  -0.297
## CURL       0.605  -0.158  -0.270
## MAXPUSHU   0.512   0.317  -0.312
##
##                Factor1 Factor2 Factor3
## SS loadings      1.912   1.545   1.243
## Proportion Var   0.212   0.172   0.138
## Cumulative Var   0.212   0.384   0.522
```

```
##  if we don't consider any rotation is different to interpret the factors.try
##  to rotate
(ml4 <- factanal(x, factors = 3, rotation = "varimax"))
```

```
##
## Call:
## factanal(x = x, factors = 3, rotation = "varimax")
##
## Uniquenesses:
##   PINBALL  BILLIARD      GOLF   X.1500M   X.2KROW X.12MINTR     BENCH      CURL
##     0.635     0.414     0.455     0.361     0.520     0.538     0.302     0.536
##  MAXPUSHU
##     0.540
##
## Loadings:
##           Factor1 Factor2 Factor3
## PINBALL            0.131   0.590
## BILLIARD                   0.765
## GOLF                       0.735
## X.1500M    0.779  -0.179
## X.2KROW    0.585   0.372
## X.12MINTR  0.678
## BENCH     -0.119   0.816   0.137
## CURL               0.674
## MAXPUSHU   0.433   0.522
```

```
##
##                Factor1 Factor2 Factor3
## SS loadings      1.613   1.584   1.502
## Proportion Var   0.179   0.176   0.167
## Cumulative Var   0.179   0.355   0.522
##
## Test of the hypothesis that 3 factors are sufficient.
## The chi square statistic is 12.94 on 12 degrees of freedom.
## The p-value is 0.373
```

```
ml4$loadings
```

```
##
## Loadings:
##           Factor1 Factor2 Factor3
## PINBALL            0.131   0.590
## BILLIARD                   0.765
## GOLF                       0.735
## X.1500M    0.779  -0.179
## X.2KROW    0.585   0.372
## X.12MINTR  0.678
## BENCH     -0.119   0.816   0.137
## CURL               0.674
## MAXPUSHU   0.433   0.522
##
##                Factor1 Factor2 Factor3
## SS loadings      1.613   1.584   1.502
## Proportion Var   0.179   0.176   0.167
## Cumulative Var   0.179   0.355   0.522
```

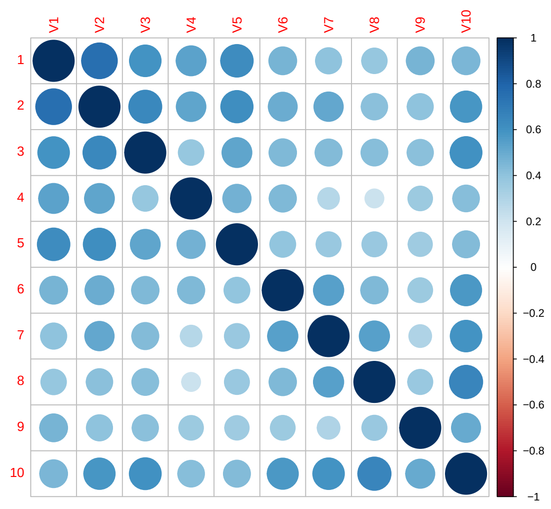
```
## to ease interpretation is to use cutoff that are in absolute value larger
## than given

print(ml4$loadings, cutoff = 0.2, digits = 2)
```

```
##
## Loadings:
##           Factor1 Factor2 Factor3
## PINBALL                    0.59
## BILLIARD                   0.76
## GOLF                       0.73
## X.1500M    0.78
## X.2KROW    0.58    0.37
## X.12MINTR  0.68
## BENCH              0.82
## CURL               0.67
## MAXPUSHU   0.43    0.52
##
##                Factor1 Factor2 Factor3
## SS loadings       1.61    1.58    1.50
## Proportion Var    0.18    0.18    0.17
## Cumulative Var    0.18    0.36    0.52

# interpretation becomes simpler: what we can see is tat the first factror has
# high entries for 1500M, 2KROW, 12mintr: it seems high ability in
# endurance/long sports variable

## second has high entries on the last three variables: it represent the
## strenght

## third factor has high entry on first three var: ability/coordination sport
## variable.

## this seems reasonable looking at correlation matrix
```

```
## -----------------------------------------
## --- now we extract the individual scores, having the dataset

## to do that
ml4reg <- factanal(x, factors = 3, rotation = "varimax", scores = "regression")
ml4bartlett <- factanal(x, factors = 3, rotation = "varimax", scores = "Bartlett")

## so now we have
head(ml4reg$scores)  # thompson: three factors

##          Factor1    Factor2     Factor3
## [1,] -0.64603135  0.5977488 -0.84052831
## [2,]  0.49077147 -0.1613787 -0.62070762
## [3,] -0.65306886 -0.9381925  0.73428198
## [4,] -0.02753535 -1.1794956  0.72268612
## [5,]  0.77251893  0.7731299  0.09496591
## [6,] -0.13301869 -0.0815587  0.38041785

head(ml4bartlett$scores) # bartlett: three factors

##          Factor1    Factor2     Factor3
## [1,] -0.81502246  0.8108272 -1.14286314
## [2,]  0.63677933 -0.1655105 -0.81955237
## [3,] -0.84449897 -1.2332453  1.04223966
## [4,] -0.04397501 -1.5387752  1.03323686
## [5,]  0.98562377  0.9715071  0.06573472
## [6,] -0.17546122 -0.1272071  0.51134257

## individuals which received highest score in sport about strenght

ord_scores <- order(ml4reg$scores[, 2], decreasing = TRUE) # second column is the str
head(ml4reg$scores[ord_scores, ])

##         Factor1  Factor2    Factor3
## [1,] -1.7772648 2.766277  1.1874676
## [2,]  0.4050792 2.603599  0.4903824
## [3,] -1.8201313 2.496708  0.6917442
## [4,]  1.4779385 2.339539 -0.5901477
## [5,]  1.0552924 2.279670  0.3561006
## [6,]  0.7579529 2.187697 -0.3514164
```

4.14 Last exercise

```
# intel dataset
x <- read.table("data/intel_test.txt") # it is a correlation matrix. do as the first
# exercise
R <- as.matrix(x)
R

##          V1    V2    V3    V4    V5    V6    V7    V8    V9   V10
##  [1,] 1.000 0.755 0.592 0.532 0.627 0.460 0.407 0.387 0.461 0.459
##  [2,] 0.755 1.000 0.644 0.520 0.617 0.497 0.511 0.417 0.406 0.583
##  [3,] 0.592 0.644 1.000 0.388 0.529 0.449 0.436 0.428 0.412 0.602
##  [4,] 0.532 0.528 0.388 1.000 0.475 0.442 0.280 0.214 0.361 0.424
##  [5,] 0.627 0.617 0.529 0.475 1.000 0.398 0.373 0.372 0.350 0.433
##  [6,] 0.460 0.497 0.449 0.442 0.398 1.000 0.545 0.446 0.366 0.575
##  [7,] 0.407 0.511 0.436 0.280 0.373 0.545 1.000 0.542 0.308 0.590
##  [8,] 0.387 0.417 0.428 0.214 0.372 0.446 0.542 1.000 0.375 0.654
##  [9,] 0.461 0.406 0.412 0.361 0.355 0.366 0.308 0.375 1.000 0.502
## [10,] 0.459 0.583 0.602 0.424 0.433 0.575 0.590 0.654 0.502 1.000

## 75 children in intelligence test
## V1: information
## V2 vocabulary
## ....

## è lo stesso dataset visto con la prof?

corrplot(R)
```



```
(ml1 <- factanal(covmat = R, factors = 2, n.obs = 75, rotation = 'none'))

##
## Call:
## factanal(factors = 2, covmat = R, n.obs = 75, rotation = "none")
##
## Uniquenesses:
##    V1    V2    V3    V4    V5    V6    V7    V8    V9   V10
## 0.215 0.249 0.452 0.622 0.482 0.553 0.534 0.481 0.679 0.177
##
## Loadings:
##       Factor1 Factor2
##  [1,]  0.789  -0.403
##  [2,]  0.834  -0.234
##  [3,]  0.740
##  [4,]  0.587  -0.185
##  [5,]  0.676  -0.247
##  [6,]  0.654   0.140
##  [7,]  0.641   0.235
##  [8,]  0.630   0.351
##  [9,]  0.564
## [10,]  0.807   0.414
##
##                Factor1 Factor2
## SS loadings      4.872   0.685
## Proportion Var   0.487   0.069
## Cumulative Var   0.487   0.556
##
## Test of the hypothesis that 2 factors are sufficient.
## The chi square statistic is 16.51 on 26 degrees of freedom.
## The p-value is 0.923
```

```
# p.val very high: two factors are enough to explain correlation of this data

ml1$uniquenesses

##        V1        V2        V3        V4        V5        V6        V7        V8
## 0.2147868 0.2492602 0.4516243 0.6217758 0.4822172 0.5528077 0.5338987 0.4806868
##        V9       V10
## 0.6790751 0.1769536

ml1$loadings

##
## Loadings:
##       Factor1 Factor2
##  [1,]  0.789  -0.403
##  [2,]  0.834  -0.234
##  [3,]  0.740
##  [4,]  0.587  -0.185
##  [5,]  0.676  -0.247
##  [6,]  0.654   0.140
##  [7,]  0.641   0.235
##  [8,]  0.630   0.351
##  [9,]  0.564
## [10,]  0.807   0.414
##
##                Factor1 Factor2
## SS loadings      4.872   0.685
## Proportion Var   0.487   0.069
## Cumulative Var   0.487   0.556
```

when we dont' perform rotation: the first factor has high entries for all the variables (its an average measurmente) while the other are contrasts.

```
(ml2 <- factanal(covmat = R, factors = 2, n.obs = 75, rotation = 'varimax'))

##
## Call:
## factanal(factors = 2, covmat = R, n.obs = 75, rotation = "varimax")
##
## Uniquenesses:
##    V1    V2    V3    V4    V5    V6    V7    V8    V9   V10
## 0.215 0.249 0.452 0.622 0.482 0.553 0.534 0.481 0.679 0.177
##
## Loadings:
##       Factor1 Factor2
##  [1,] 0.852   0.245
##  [2,] 0.769   0.399
##  [3,] 0.563   0.481
##  [4,] 0.555   0.266
##  [5,] 0.662   0.281
##  [6,] 0.382   0.549
##  [7,] 0.308   0.609
##  [8,] 0.220   0.686
##  [9,] 0.375   0.424
## [10,] 0.307   0.854
##
##                Factor1 Factor2
## SS loadings      2.904   2.653
## Proportion Var   0.290   0.265
## Cumulative Var   0.290   0.556
##
## Test of the hypothesis that 2 factors are sufficient.
## The chi square statistic is 16.51 on 26 degrees of freedom.
## The p-value is 0.923

print(ml2$loadings) # first factor high on first five variables, second on last

##
## Loadings:
##       Factor1 Factor2
##  [1,] 0.852   0.245
##  [2,] 0.769   0.399
##  [3,] 0.563   0.481
##  [4,] 0.555   0.266
##  [5,] 0.662   0.281
##  [6,] 0.382   0.549
##  [7,] 0.308   0.609
##  [8,] 0.220   0.686
##  [9,] 0.375   0.424
## [10,] 0.307   0.854
##
##                Factor1 Factor2
## SS loadings      2.904   2.653
## Proportion Var   0.290   0.265
## Cumulative Var   0.290   0.556

# five variables
# vedi interpretazione poi negli appunti
```

Capitolo 5

Discriminant analysis and supervised classification

The purpose of linear discriminant analysis (LDA) is to find the linear combinations of the original variables that give the best possible separation between the groups in our data set. Linear discriminant analysis is also known as canonical discriminant analysis" or simply "discriminant analysis".

5.1 Discriminant analysis

Methods is based on *linear combinations*: aim is to find coefficients of the linear combination which is best at dividing some known groups. It's an old method, invented by Fisher in 1936, which is still very useful because it's interpretable (if we use a neural network to do the same it all become very less clear).

Suppose we have two population, Π_1 and Π_2 where we can observe a random vector $\mathbf{X}$ $(p \times 1)$ which has different mean $(\boldsymbol{\mu}_1, \boldsymbol{\mu}_2$ in the two population) but common variance/covariance $\boldsymbol{\Sigma}_1 = \boldsymbol{\Sigma}_2 = \boldsymbol{\Sigma}$ (only assumptions Fisher made was homoscedasticity).
We draw a sample from the two population C_1 and C_2, composed by n_1 units and n_2 units respectively, with mean $\overline{\mathbf{x}}_1, \overline{\mathbf{x}}_2$ and covariances S_1, S_2 (say the unbiased version one but it is not necessary).
To separate two groups, something that often does better than original variables is a linear combination: Fisher proposed to look for the linear combination of the observed variables such that, when projected along it, the groups are maximally separated (distant means) and at the same time maximally homogeneous (variance within group is small).
He wanted to find a such as

$$y = \mathbf{a}^\top \mathbf{X}$$

the groups in y are maximally separated and homogeneous.
Fisher developed LDA, consistently with the idea of Anova, to find $\mathbf{a}$ such that when projected, variance of y between group is maximum and variance within group is minimum.
To procede we need to define (in the general case of G groups):

- the mean of y in a single group is the linear combination of the original data means

$$\begin{aligned} \overline{y}_1 &= \mathbf{a}^\top \overline{\mathbf{x}}_1 \\ \overline{y}_2 &= \mathbf{a}^\top \overline{\mathbf{x}}_2 \\ &\dots \\ \overline{y}_G &= \mathbf{a}^\top \overline{\mathbf{x}}_G \end{aligned}$$

- the overall mean is a weighted mean of the two above

$$\overline{y} = \frac{n_1\overline{y}_1 + n_2\overline{y}_2 + \dots n_G\overline{y}_G}{n_1 + n_2 + \dots + n_G} = \frac{n_1\mathbf{a}^\top\overline{\mathbf{x}}_1 + n_2\mathbf{a}^\top\overline{\mathbf{x}}_2 + \dots + n_G\mathbf{a}^\top\overline{\mathbf{x}}_G}{n}$$

5.1.1 Variance between

The *between variance* of y is the between group sum of square divided by the degrees of freedom (here G is the general number of groups, here we have two so $G = 2$)

$$V(y)_{\text{between}} = \frac{BSS}{df} = \frac{\sum_{g=1}^{G}(\overline{y}_g - \overline{y})^2 \cdot n_g}{G-1}$$

the degrees of freedom are due to G means and 1 constraint (1 grand mean): in the two group cases, $df = 1$.
To express in matrix form

$$\begin{aligned} V(y)_{\text{between}} &= \frac{1}{G-1}\sum_{g=1}^{G}(\overline{y}_g - \overline{y})^2 \cdot n_g = \frac{1}{G-1}\sum_{g=1}^{G}(\mathbf{a}^\top\overline{\mathbf{x}}_g - \mathbf{a}^\top\overline{\mathbf{x}})^2 n_g \\ &= \frac{1}{G-1}\sum_{g=1}^{G}\left[\mathbf{a}^\top(\overline{\mathbf{x}}_g - \overline{\mathbf{x}})\right]^2 n_g = \frac{1}{G-1}\sum_{g=1}^{G}\mathbf{a}^\top(\overline{\mathbf{x}}_g - \overline{\mathbf{x}})(\overline{\mathbf{x}}_g - \overline{\mathbf{x}})^T\mathbf{a}^\top n_g \\ &= \frac{1}{G-1}\mathbf{a}^\top\left[\sum_{g=1}^{G}(\overline{\mathbf{x}}_g - \overline{\mathbf{x}})(\overline{\mathbf{x}}_g - \overline{\mathbf{x}})^T \cdot n_g\right]\mathbf{a}^\top \end{aligned}$$

Now if we name the original variables between groups variance

$$\mathbf{B} = \frac{1}{G-1}\sum_{g=1}^{G}\left[(\overline{\mathbf{x}}_g - \overline{\mathbf{x}})(\overline{\mathbf{x}}_g - \overline{\mathbf{x}})^T \cdot n_g\right]$$

where $\mathbf{B}$ is the between group variance in the original X space. We can finally rewrite the variance between of y as function of variance between of $\mathbf{x}$:

$$V(y) = \mathbf{a}^\top\mathbf{B}\mathbf{a}$$

This for the general case.

Important remark 36. Now regarding $\mathbf{B}$:

- dimension of matrix $\mathbf{B}$: with p variables B is a $p \times p$ matrix

- what's its rank? In the general case has at most rank $G-1$

Thus the matrix B **is not full rank**.

Important remark 37. An alternative way to write $\mathbf{B}$, in case we have only two groups is the following

$$\begin{aligned}
V(y) &= \sum_{g=1}^{2}(\overline{y}_g - \overline{y})^2 \cdot n_g = (\overline{y}_1 - \overline{y})^2 \cdot n_1 + (\overline{y}_2 - \overline{y})^2 \cdot n_2 \\
&= n_1 \left[\mathbf{a}^\top \overline{\mathbf{x}}_1 - \frac{1}{n}\left(\mathbf{a}^\top \overline{\mathbf{x}}_1 n_1 + \mathbf{a}^\top \overline{\mathbf{x}}_2 n_2\right)\right]^2 + n_2 \left[\mathbf{a}^\top \overline{\mathbf{x}}_2 - \frac{1}{n}\left(\mathbf{a}^\top \overline{\mathbf{x}}_1 n_1 + \mathbf{a}^\top \overline{\mathbf{x}}_2 n_2\right)\right]^2 \\
&= \frac{n_1\left[n\mathbf{a}^\top \overline{\mathbf{x}}_1 - \mathbf{a}^\top \overline{\mathbf{x}}_1 n_1 - \mathbf{a}^\top \overline{\mathbf{x}}_2 n_2\right]^2}{n^2} + n_2 \frac{\left[n\mathbf{a}^\top \overline{\mathbf{x}}_2 - \mathbf{a}^\top \overline{\mathbf{x}}_1 n_1 - \mathbf{a}^\top \overline{\mathbf{x}}_2 n_2\right]^2}{n^2} \\
&= \frac{n_1}{n^2}\left(\mathbf{a}^\top \overline{\mathbf{x}}_1 n_2 - \mathbf{a}^\top \overline{\mathbf{x}}_2 n_2\right)^2 + \frac{n_2}{n^2}\left(\mathbf{a}^\top \overline{\mathbf{x}}_2 n_1 - \mathbf{a}^\top \overline{\mathbf{x}}_1 n_1\right)^2 \\
&= \frac{n_1 n_2^2}{n^2}\left[\mathbf{a}^\top(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)\right]^2 + \frac{n_2 n_1^2}{n^2}\left[\mathbf{a}^\top(\overline{\mathbf{x}}_2 - \overline{\mathbf{x}}_1)\right]^2 \\
&= \frac{n_1 n_2^2}{n^2}\mathbf{a}^\top(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)^\top \mathbf{a} + \frac{n_1^2 n_2}{n^2} a^\top(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)^\top \mathbf{a} \\
&= \frac{n_1 n_2^2 + n_1^2 n_2}{n^2}\mathbf{a}^\top(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)^\top \mathbf{a} \\
&\overset{(1)}{=} \frac{n_1 \cdot n_2}{n_1 + n_2}\mathbf{a}^\top(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)^\top \mathbf{a}
\end{aligned}$$

where in (1) we simplified using $n^2 = (n_1 + n_2)^2$.
So in the two groups cases here we have that

$$\mathbf{B} = \frac{n_1 \cdot n_2}{n_1 + n_2}(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)^\top$$

Remark 24. In the two groups case $\mathbf{B}$ is the product of the col vector times row vector: the product is rank 1 (since both row and col vector has rank 1). So in case of in the case of two group $\mathbf{B}$ has rank 1.

5.1.2 Variance within

Now let's check variance within, that is the sum of variances withing group. Using the unbiased estimator (here below $\mathbf{x}_g$ are the units from group g)

$$\begin{aligned}
V(y)_{\text{within}} &= \frac{\sum_{g=1}^{G} \operatorname{Var}[y_g](n_g - 1)}{n - G} = \frac{\sum_{g=1}^{G} \operatorname{Var}\left[\mathbf{a}^T \mathbf{x}_g\right](n_g - 1)}{n - G} \\
&= \frac{\sum_{g=1}^{G} \mathbf{a}^T \operatorname{Var}[\mathbf{x}_g]\,\mathbf{a} \cdot (n_g - 1)}{n - G} \overset{(1)}{=} \frac{\sum_{g=1}^{G} \mathbf{a}^T \mathbf{S}_g \mathbf{a} \cdot (n_g - 1)}{n - G} \\
&= \mathbf{a}^T \left[\frac{\sum_{g=1}^{G} \mathbf{S}_g (n_g - 1)}{n - G}\right] \mathbf{a} \\
&= \mathbf{a}^T \mathbf{W} \mathbf{a}
\end{aligned}$$

where in (1) we used $\operatorname{Var}[aX] = a^2 \operatorname{Var}[X]$ and $\mathbf{W}$ is the within group sum of square for x.

Remark 25. Now we rephrased within and between variance in terms of **a** so we can choose **a** optimizing.

Important remark 38 (Recap). Only assumption so far is that the G population shares covariance matrix (not any hypothesis on shape of distribution) and ended finding the variances of linear combination with **a**, which are

$$\begin{aligned} V(Y)_b &= \mathbf{a}^\top \mathbf{B}\mathbf{a} \\ V(Y)_w &= \mathbf{a}^\top \mathbf{W}\mathbf{a} \end{aligned}$$

with **B** and **W** the between and within group variance in the x space. Now we have what needed to derive Fisher criterion.

5.1.3 Fisher's criterion

Fisher wanted to find a linear combination $y = \mathbf{a}^\top X$ such that the ratio

$$\phi = \frac{V(y)_b}{V(y)_w} = \frac{\mathbf{a}^\top \mathbf{B}\mathbf{a}}{\mathbf{a}^\top \mathbf{W}\mathbf{a}}$$

is maximum with respect to **a**; this means a combination which creates groups that are mostly separated (max variance at the numerator num) and homogeneous (min variance denominator). So our problem is $\max_{\mathbf{a}} \phi$, a standard maximum problem; we derive wrt to **a** and equate to 0

$$\begin{aligned} \frac{\partial \phi}{\partial \mathbf{a}} &= \frac{2\mathbf{B}\mathbf{a}(\mathbf{a}^\top \mathbf{W}\mathbf{a}) - 2\mathbf{W}\mathbf{a}(\mathbf{a}^\top \mathbf{B}\mathbf{a})}{(\mathbf{a}^\top \mathbf{W}\mathbf{a})^2} = 2\left[\frac{\mathbf{B}\mathbf{a}(\mathbf{a}^\top \mathbf{W}\mathbf{a})}{(\mathbf{a}^\top \mathbf{W}\mathbf{a})^2} - \frac{\mathbf{W}\mathbf{a}(\mathbf{a}^\top \mathbf{B}\mathbf{a})}{(\mathbf{a}^\top \mathbf{W}\mathbf{a})^2}\right] \\ &\overset{(1)}{=} 2\left[\frac{\mathbf{B}\mathbf{a}}{\mathbf{a}^\top \mathbf{W}\mathbf{a}} - \frac{\mathbf{W}\mathbf{a}\phi}{\mathbf{a}^\top \mathbf{W}\mathbf{a}}\right] \end{aligned}$$

where in (1) we just replaced $\frac{a^\top Ba}{a^\top Wa} = \phi$. Furthermore $\mathbf{a}^\top \mathbf{W}\mathbf{a}$ is a constant $\neq 0$; by equating to 0 for maximization we can simplify to

$$\begin{aligned} \mathbf{B}\mathbf{a} - \phi \mathbf{W}\mathbf{a} &= \mathbf{0} \\ (\mathbf{B} - \phi \mathbf{W})\mathbf{a} &= \mathbf{0} \end{aligned}$$

Now we premultiply both sides by $\mathbf{W}^{-1}$ (under the assumption that **W** it is non singular)

$$\left(\mathbf{W}^{-1}\mathbf{B} - \phi \mathbf{I}\right)\mathbf{a} = \mathbf{0}$$

This last is a linear equation system which admits a nontrivial solution iff the determinant

$$\det\left(\mathbf{W}^{-1}\mathbf{B} - \phi \mathbf{I}\right) = 0$$

that is if ϕ is a root of the characteristics polynomial of $\mathbf{W}^{-1}\mathbf{B}$. This means that ϕ is an eigenvalue of $\mathbf{W}^{-1}\mathbf{B}$ and **a** is the corresponding eigenvector. If we prefer we can rewrite as the eigenvalue eigenvector relationship

$$(\mathbf{W}^{-1}\mathbf{B} - \phi \mathbf{I})\mathbf{a} = \mathbf{0} \implies \mathbf{W}^{-1}\mathbf{B}\mathbf{a} = \phi \mathbf{a}$$

Important remark 39. How many non zero eigenvalue do we have? the rank of $\mathbf{W}^{-1}\mathbf{B}$

- in the two group cases: the rank of $\mathbf{W}$ is p, while $\mathbf{B}$ is $p \times p$ matrix but its rank is 1. So the product $\mathbf{W}^{-1}\mathbf{B}$ will have rank 1: therefore it will have just 1 non zero eigenvalue.
  In the 2 group cases the **best linear discriminant direction** will be the *eigenvector* of $\mathbf{W}^{-1}\mathbf{B}$ corresponding to the non zero eigenvalue

- in the general G group case: the rank $\mathbf{W}^{-1}\mathbf{B}$ will be at most $G-1$, so will have at most $G-1$ non null eigenvalue and at most $G-1$ discriminant directions (indipendently from how large is p eg I can have 100 variables).
  The optimal linear discriminant direction will be defined by the *eigenvector* of $W^{-1}B$ corresponding to the *largest eigenvalue* as ϕ.
  In this case we can consider more than 1 discriminant directions: we can consider the *eigenvector corresponding to different eigenvalues in decreasing order* (each of them will have a decreasing discrimination power). [1].
  These eigenvector

  - define a vector subspace containing te variability between features;
  - are primarily used in feature reduction and can be interpreted in the same way as principal compoennts

Remark 26. Fisher proved that in the two group case, the eigenvector of $\mathbf{W}^{-1}\mathbf{B}$ corresponding to the only non zero eigenvalues can be obtained in closed form as

$$\mathbf{a} = \mathbf{W}^{-1}(\overline{x}_1 - \overline{x}_2)$$

5.1.4 Differences with PCA

Important remark 40. So we're again trying to solve a linear equations system as done for principal components. The differences with Principal components:

1. here we don't need any constraint (there we needed to constraint a to have norm 1) because it appears both at numerator and denominator

   TODO: cosa? riascolta

2. while the covariance matrix $\mathbf{S}, \mathbf{\Sigma}$ is symmetric, this matrix $\mathbf{W}^{-1}\mathbf{B}$ is non-symmetric (it's the produt of two symmetric matrices but it is not). Spectral decomposition exists but there can be immaginary eigenvalue/vectors

3. it can be that LDA outperform PCA in classification: discriminatory information is not necessary aligned with the direction of maximum variability

[1]eg if we have three groups we can go on and find the second discriminant direction corresponding to the second highest larger eigenvalue

5.1.5 Linear discriminant functions

The linear combinations:

$$\begin{aligned} y_1 &= \mathbf{a}_1^\top \mathbf{x} \\ y_2 &= \mathbf{a}_2^\top \mathbf{x} \\ &\dots \\ y_{G-1} &= \mathbf{a}_{G-1}^\top \mathbf{x} \end{aligned}$$

with $\mathbf{a}_1, \dots, \mathbf{a}_{G-1}$ the eigenvectors corresponding to the non zero eigenvalues in decreasing order, are called linear *discriminant functions* (or also *canonical variates*).

5.1.6 Correlation of eigenvectors

Lets' consider two different discriminant directions $\mathbf{a}_i, \mathbf{a}_j$ and their corresponding eigengector ϕ_i, ϕ_j. Being solution we have that hold:

$$\begin{aligned} \mathbf{B}\mathbf{a}_i &= \phi_i \mathbf{W}\mathbf{a}_i \\ \mathbf{B}\mathbf{a}_j &= \phi_j \mathbf{W}\mathbf{a}_j \end{aligned}$$

Let's pre multiply the first by $\mathbf{a}_j^\top$ and the second by $\mathbf{a}_i^\top$

$$\begin{aligned} \mathbf{a}_j^\top \mathbf{B}\mathbf{a}_i &= \phi_i \mathbf{a}_j^\top \mathbf{W}\mathbf{a}_i \\ \mathbf{a}_i^\top \mathbf{B}\mathbf{a}_j &= \phi_j \mathbf{a}_i^\top \mathbf{W}\mathbf{a}_j \end{aligned}$$

On the left hand side of the two equations we have two quantities that are the same: two scalar which is one the transpose of the other (transpose of scalar is the scalar itself), that is

$$\mathbf{a}_j^\top \mathbf{B}\mathbf{a}_i = \mathbf{a}_i^\top \mathbf{B}\mathbf{a}_j$$

thus event the right hand side has to be the same as well

$$\phi_i \mathbf{a}_j^\top \mathbf{W}\mathbf{a}_i = \phi_j \mathbf{a}_i^\top \mathbf{W}\mathbf{a}_j$$

and we have that even $\mathbf{a}_j^\top \mathbf{W}\mathbf{a}_i = \mathbf{a}_i^\top \mathbf{W}\mathbf{a}_j$ for the same reason before (a scalar and its equivalent transpose). Now:

- Given that ϕ_i and ϕ_j are different from zero, and different each other, in order for the equality to hold it must be that

  $$\mathbf{a}_j^\top \mathbf{W}\mathbf{a}_i = \mathbf{a}_i^\top \mathbf{W}\mathbf{a}_j = 0$$

  Now if we put all the discriminant direction together in the matrix $\mathbf{A}$ we have that

  $$\mathbf{A}^\top \mathbf{W}\mathbf{A} \quad \text{is diagonal}$$

  because crossproducts have to be all equal to 0.
  This means that **discriminant directions are uncorrelated within group**: as $\mathbf{a}_i^\top \mathbf{W}\mathbf{a}_j$ is the covariance between y_i and y_j within group (there's $\mathbf{W}$), then we conclude that the linear discriminant functions are uncorrelated within groups.

- having said that
$$\mathbf{a}_i^\top \mathbf{W}\mathbf{a}_j = 0 \implies \mathbf{a}_i^\top \mathbf{B}\mathbf{a}_j = 0$$
so it means that the discriminant function are **uncorrelated also between groups**.

- If they are uncorrelated both within and between groups, they are overall uncorrelated, with respect to the whole set of units, so this means that $\mathbf{A}^\top \mathbf{S}\mathbf{A}$ is diagonal.
This is one important difference we'have not asked for: the orthogonality.

Remark 27. Many softwares (R included) scale $\mathbf{A}$ so that $\mathbf{A}^\top \mathbf{W}\mathbf{A}$ not only is diagonal but $\mathbf{A}^\top \mathbf{W}\mathbf{A} = \mathbf{I}$ (the discriminant variables are uncorrelated and have unit within group variance; they're often said to be sphered

5.1.7 Example: iris

Example 5.1.1 (Fisher's Iris Data)**.** We have data on 150 iris flowers belonging to three species (setosa, versicolor and verginica); for each flower the length and width of the flower and sepal length and width. The group means are

$$\begin{aligned}\overline{\mathbf{x}}_1^T &= \begin{bmatrix}5.006 & 3.418 & 1.464 & 0.244\end{bmatrix}\\ \overline{\mathbf{x}}_2^T &= \begin{bmatrix}5.936 & 2.77 & 4.26 & 1.326\end{bmatrix}\\ \overline{\mathbf{x}}_3^T &= \begin{bmatrix}6.558 & 2.974 & 5.552 & 2.026\end{bmatrix}\end{aligned}$$

we have three groups, we expect to find two discriminant directions, which respectively correspond to eigenvalue $\phi_1 = 32.27$ and $\phi_2 = 0.278$

$$\begin{aligned}\mathbf{a}_1^T &= \begin{bmatrix}-0.2048 & 0.3871 & -0.5465 & -0.7138\end{bmatrix}\\ \mathbf{a}_2^T &= \begin{bmatrix}-0.008 & -0.589 & 0.2543 & -0.767\end{bmatrix}\end{aligned}$$

The obtained projected of the first LD for the three groups are respectively $\overline{\mathbf{y}}_{11} = 1.37$ (setosa) $\overline{\mathbf{y}}_{21} = -0.98$ (virsicolor) $\overline{\mathbf{y}}_{31} = -1.98$ (virginica)

- looking at the variables: the first direction separates flower with big sepal and low petal and viceversa
- the second direction $\mathbf{a}_2^\top$ is focused on sepal only

The projection on LD1 and LD2: setosa is most separated on the first LD1 while on the second there's not too much separation. Separation on first is good

5.2 Performing classification

5.2.1 Using LDA

Remark 28. Even if it has been derived for discrimination purposes, Fisher's linear function can also be used to address classification issues, i.e. to define a rule for assigning a unit, whose group membership is unknown, to one out of the G groups.
The method is general, but for teaching purposes we will limit our attention to the two group case only.

In the two groups cases: I have data $\mathbf{x}_0$ on a new unit (a $p \times 1$ vector) whose membership is unknown. Data includes the same variables I have used to obtain the discriminant function. I can calculate

$$y_0 = \mathbf{a}^\top \mathbf{x}_0$$

where $\mathbf{a}$ is the discriminant direction. In the two group case I also compute the projection of the mean of groups $(\overline{\mathbf{x}}_1, \overline{\mathbf{x}}_2)$ along $\mathbf{a}$

$$\overline{y}_2 = \mathbf{a}^\top \overline{\mathbf{x}}_2 \qquad\qquad \overline{y}_1 = \mathbf{a}^\top \overline{\mathbf{x}}_1$$

Assuming for simplicity that $\overline{y}_1 > \overline{y}_2$, to classify my unit I project it on the discriminant direction (calculating y_0) and check the distance between the projection and the means projected

$$\begin{aligned} |y_0 - \overline{y}_2| < |y_0 - \overline{y}_1| &\implies \mathbf{x}_0 \in \Pi_2 \\ |y_0 - \overline{y}_1| < |y_0 - \overline{y}_2| &\implies \mathbf{x}_0 \in \Pi_1 \end{aligned}$$

Alternatively said:

$$\begin{cases} y_0 > \frac{\overline{y}_1 + \overline{y}_2}{2} & \implies \mathbf{x}_0 \in \Pi_1 \\ y_0 < \frac{\overline{y}_1 + \overline{y}_2}{2} & \implies \mathbf{x}_0 \in \Pi_2 \\ y_0 = \frac{\overline{y}_1 + \overline{y}_2}{2} & \implies \text{toss a coin to decide which group} \end{cases}$$

In the two group case, as said previously, Fisher proved that the eigenvector of $\mathbf{W}^{-1}\mathbf{B}$ corresponding to the only direction $\mathbf{a}$ be obtained in closed form as:

$$\mathbf{a} = \mathbf{W}^{-1}(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)$$

By exploiting this we can say

$$y_0 = \mathbf{a}^\top \mathbf{x}_0 = (\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)^\top \mathbf{W}^{-1} \mathbf{x}_0$$

where being $\mathbf{W}$ symmetric, it's transpose coincides with the inverse. The group transformed means become

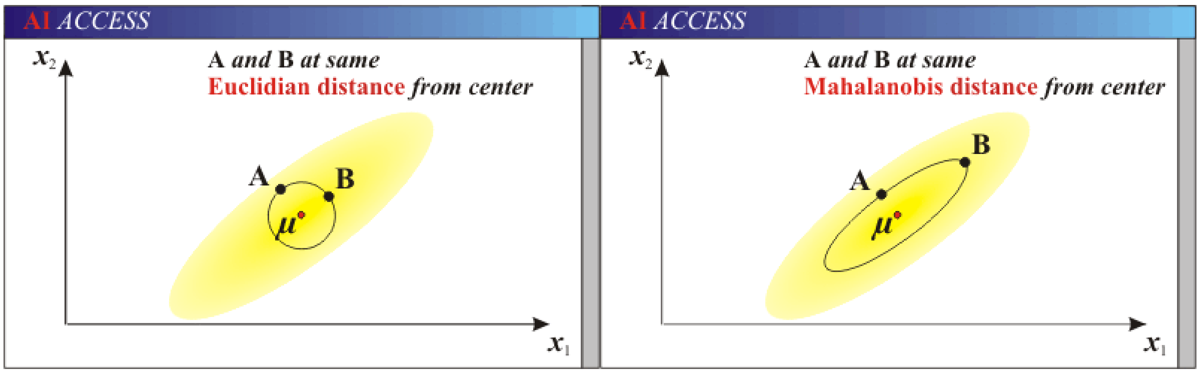
$$\begin{aligned} \overline{y}_1 &= \mathbf{a}^\top \overline{\mathbf{x}}_1 = (\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)^\top \mathbf{W}^{-1} \overline{\mathbf{x}}_1 \\ \overline{y}_2 &= \mathbf{a}^\top \overline{\mathbf{x}}_2 = (\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)^\top \mathbf{W}^{-1} \overline{\mathbf{x}}_2 \end{aligned}$$

So the rule to assign $\mathbf{x}_0$ in Π_1, becomes

$$\begin{aligned} & y_0 > \frac{\overline{\mathbf{y}}_1 + \overline{\mathbf{y}}_2}{2} \\ & (\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)^\top \mathbf{W}^{-1} \mathbf{x}_0 > \frac{1}{2} (\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)^\top \mathbf{W}^{-1} (\overline{\mathbf{x}}_1 + \overline{\mathbf{x}}_2) \end{aligned} \tag{5.1}$$

This last is called **Fisher 's linear discriminant** classification rule.

Remark 29. This allocation rule is very popular as it can be obtained addressing the classification problem according to a variety of different perspectives. We will see a couple of them in the following.



(a) (b)

Figura 5.1: Euclidean and Mahalanobis distance

5.2.2 Using Mahalanobis distance

Remark 30. Classification problem can be addressed directly in the original p-dimensional space by assigning a unit (whose group membership is unknown) to the population from which it has the smallest Mahalanobis distance (from the mean).

5.2.2.1 The Mahalanobis distance

One common way to measure the distance between points in a p dimensional space is provided by the **Euclidean distance**; however it attaches equal weight to all the axes of the representation.
If differences are present in the variances of the observed variables, and if the variables are correlated this might not be a desirable feature.
In Fig.5.1 a bivariate point cloud is represented: The variables have different variances and are correlated. The points A and B have the same Euclidean distance from the center of the point cloud (i.e. from the average vector) but while B lies in the core of the distribution, A is in a low frequency region.

Mahalanobis distance provides a way to take into account variances and correlations when computing distances, i.e. to take into account the shape of the point cloud. Given a point whose coordinate vector is $\mathbf{x}$, its Mahalonobis distance from the center of the point cloud $\overline{\mathbf{x}}$ is defined as

$$d_M(\mathbf{x}, \overline{\mathbf{x}}) = \sqrt{(\mathbf{x} - \overline{\mathbf{x}})^\top \mathbf{S}^{-1} (\mathbf{x} - \overline{\mathbf{x}})}$$

where as usual, $\mathbf{S}$ is the sample covariance matrix. Mahalanobis distance is thus a weighted Euclidean distance. In Fig.5.1 the same point cloud and two points having the same Mahalanobis distance are represented.

Important remark 41. Mahalanobis is a special kind, actually weighted, of euclidean distance (which consider the covariance/correlation of two variables). This can be seen by the fact that if we substitute $\mathbf{S}^{-1}$ with $\mathbf{I}$ we obtain the euclidean distance: actually Mahalanobis is a weighted euclidean distance, has an inverse covariance matrix in between.

5.2.2.2 Using it for classification

Mahalanobis distance turns out to be really useful also for classification purposes. Assuming homoscedasticity, and estimating the unknown common covariance matrix by the within group covariance matrix $\mathbf{W}$, the *squared* distances between a unit $\mathbf{x}_0$ and groups means:

$$(\mathbf{x}_0 - \overline{\mathbf{x}}_1)^\top \mathbf{W}^{-1}(\mathbf{x}_0 - \overline{\mathbf{x}}_1)$$
$$(\mathbf{x}_0 - \overline{\mathbf{x}}_2)^\top \mathbf{W}^{-1}(\mathbf{x}_0 - \overline{\mathbf{x}}_2)$$

So the rule to assign to Π_1 becomes

$$(\mathbf{x}_0 - \overline{\mathbf{x}}_1)^\top \mathbf{W}^{-1}(\mathbf{x}_0 - \overline{\mathbf{x}}_1) < (\mathbf{x}_0 - \overline{\mathbf{x}}_2)^\top \mathbf{W}^{-1}(\mathbf{x}_0 - \overline{\mathbf{x}}_2)$$
$$\mathbf{x}_0^\top \mathbf{W}^{-1}\mathbf{x}_0 - \overline{\mathbf{x}}_1^\top \mathbf{W}^{-1}\mathbf{x}_0 - \mathbf{x}_0^\top \mathbf{W}^{-1}\overline{\mathbf{x}}_1 + \overline{\mathbf{x}}_1^\top \mathbf{W}^{-1}\overline{\mathbf{x}}_1 < \mathbf{x}_0^\top \mathbf{W}^{-1}\mathbf{x}_0 - \mathbf{x}_2^\top \mathbf{W}^{-1}\mathbf{x}_0 - \mathbf{x}_0^\top \mathbf{W}^{-1}\overline{\mathbf{x}}_2 + \overline{\mathbf{x}}_2^\top \mathbf{W}^{-1}$$

now

- we simplify the first two terms ($\mathbf{x}_0^\top \mathbf{W}^{-1}\mathbf{x}_0$) in both members of inequality
- note that $\overline{\mathbf{x}}_1^\top \mathbf{W}^{-1}\mathbf{x}_0$ is a constant, transpose of $\mathbf{x}_0^T \mathbf{W}^{-1}\overline{\mathbf{x}}_1$, so coincides with it and we gather/put together
- same happens for $\overline{\mathbf{x}}_2^\top \mathbf{W}^{-1}\mathbf{x}_0$ and $\mathbf{x}_0^\top \mathbf{W}^{-1}\overline{\mathbf{x}}_2$ are

Thus:

$$-2\overline{\mathbf{x}}_1 \mathbf{W}^{-1}\mathbf{x}_0 + \overline{\mathbf{x}}_1^\top \mathbf{W}^{-1}\overline{\mathbf{x}}_1 < -2\overline{\mathbf{x}}_2 \mathbf{W}^{-1}\mathbf{x}_0 + \overline{\mathbf{x}}_2^\top \mathbf{W}^{-1}\overline{\mathbf{x}}_2$$
$$2\overline{\mathbf{x}}_1^\top \mathbf{W}^{-1}\mathbf{x}_0 - 2\overline{\mathbf{x}}_2 \mathbf{W}^{-1}\mathbf{x}_0 > \overline{\mathbf{x}}_1^\top \mathbf{W}^{-1}\overline{\mathbf{x}}_1 - \mathbf{x}_2 \mathbf{W}^{-1}\overline{\mathbf{x}}_2$$

at the second member we have a difference of two squares. By gathering, we end with the same rule as Fisher's one:

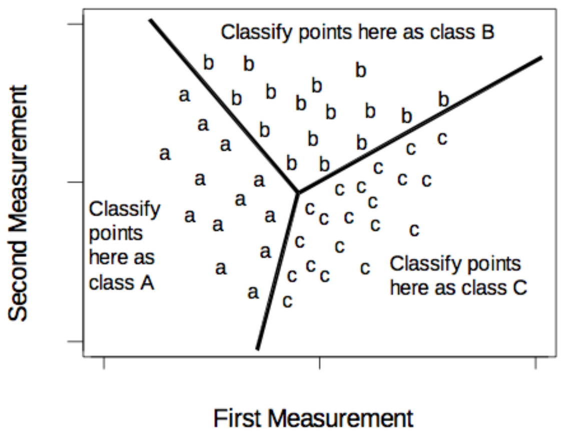
$$(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)^\top \mathbf{W}^{-1}\mathbf{x}_0 > \frac{1}{2}(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)^\top \mathbf{W}^{-1}(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2) \qquad (5.2)$$

Important remark 42. So assigning a unit to the population it is closest to in the linear discriminant space is the same as assigning the unit to the populationo which it has the smallest Mahalanobis distance in the original p-dimensional space.

Remark 31. Ine final comment: in the linear discriminant space the linear discriminant function are uncorrelated (so we don't need a weight that accounts for correlation).
Thus using Mahalanobis is original space is same as using euclidean in the transformed space.

Important remark 43. The method can be extended to the classification of units into more than 2 groups (5.2). In the G group case we allocate an object to the group for which either

- (a) the Mahalanobis distance between the object and the class mean is smallest using the original variables or
- (b) the Euclidean distance between the object and the class mean is in the subspace spanned by the Canonical Variates



(a)

Figura 5.2: Classification with three groups and mahalanobis distance

5.2.3 Classification based on probability models

So far we have addressed classification issues in a purely distribution free context. Now we will assume that we know the shape of the probability density functions (pdf) that have generated our data in the G groups. We will consider the $G = 2$ case only.
Let:

- $\mathbf{x}$ be the p-dimensional vector of the observed variables
- we call R the sample space: set of all the possible values that $\mathbf{x}$ can take;
- $\mathbf{x}_0$ a new unit whose group membership is unknown
- Π_1, Π_2 the two populations to which either it can belong
- we assume to know the density of the two populations

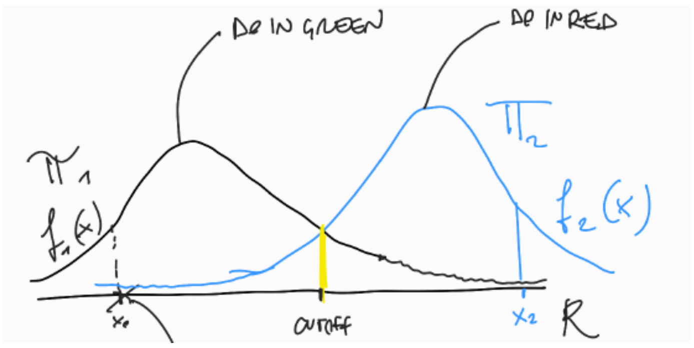
$$f(\mathbf{x}|\mathbf{x} \in \Pi_1) = f_1(\mathbf{x})$$
$$f(\mathbf{x}|\mathbf{x} \in \Pi_2) = f_2(\mathbf{x})$$

The key assumption is that x has a different pdf in Π_1 and Π_2. As $f_1(\mathbf{x})$ and $f_2(\mathbf{x})$ usually overlap, each point of R can belong both to Π_1 and Π_2, but with a different probability degree

The goal is to partition R into two regions R_1 and R_2 (mutually exclusive and exaustive, that is $R_1 \cup R_2 = R$ and $R_1 \cap R_2 = \emptyset$) such that that

- if $\mathbf{x}_0$ falls in R_1 it is assigned to population Π_1
- if $\mathbf{x}_0$ falls in R_2 it is assigned to Π_2 and
- probability of a wrong assignment is minimized

Once found the split in R_1 and R_2 it can be used to classify.



(a)

Figura 5.3: Two densities

5.2.3.1 Two population with same prior probability

assume we've two population with densities as depicted in figure 5.3: populations are not perfectly separated, tails overlap, the two population shares a part of the domain. We want to split the domain R:

- in case of the $\mathbf{x}_0$ on the figure it is more likely that the unit comes from Π_1 than Π_2. so I assign it to Π_1
- in case of $\mathbf{x}_2$ it is more liklely that the unit comes from Π_2 than from Π_1, so I assign it to Π_2
- the cutoff between the two population will be at the cross of the two curves in yellow. the split is with R_1 to the left and R_2 on the right

All above far can be translated in a very simple classification rule:

$$\frac{f_1(\mathbf{x}_0)}{f_2(\mathbf{x}_0)} > 1 \implies \mathbf{x}_0 \in \Pi_1$$

because it's more likely that $\mathbf{x}_0$ comes from population 1 than if it comes from population 2. The partition (and classifier associated) would be:

$$\begin{aligned} R_1 &= \left\{ \mathbf{x}_0 : \frac{f_1(\mathbf{x}_0)}{f_2(\mathbf{x}_0)} > 1 \right\} \\ R_2 &= \left\{ \mathbf{x}_0 : \frac{f_1(\mathbf{x}_0)}{f_2(\mathbf{x}_0)} < 1 \right\} \\ \text{toss a coin if } & \left\{ x : \frac{f_1(\mathbf{x}_0)}{f_2(\mathbf{x}_0)} = 1 \right\} \end{aligned}$$

So finally, assuming I know the distributions f_1, f_2, I can compute the likelihood of the data, and then the ratio of likelihood and finally choose.
This rule is **likelihood ratio rule** (f_1 and f_2 plays the role of likelihood).

5.2.3.2 Two population with different prior probability

Things are not always so simple: it can be that not all population are equally likely have the same a priori probability (eg rare disease common disease we need to take in account). Now let:

- π_1 to be the prior probability that a unit comes from population 1
- π_2 to be the prior probability that a unit comes from population 2
- $\pi_1 + \pi_2 = 1$

The total probability of a wrong classification p is:

$$p = p(1|2) + p(2|1)$$

that is the sum of probability that I assign a unit to population 1 when it comes from population 2 and the viceversa. This two kind of mistake could have different probabilities which are

$$\begin{aligned} p(2|1) &= \pi_1 \int_{R_2} f_1(\mathbf{x}) \, \mathrm{d}\mathbf{x} \\ p(1|2) &= \pi_2 \int_{R_1} f_2(\mathbf{x}) \, \mathrm{d}\mathbf{x} \end{aligned}$$

where, eg $\int_{R_2} f_1(\mathbf{x}) \, \mathrm{d}\mathbf{x}$ is the probability of being wrongly classified in population 2 for those who belong to population 1. Thus the total probability of a wrong classification becomes

$$p = \pi_1 \int_{R_2} f_1(\mathbf{x}) \, \mathrm{d}\mathbf{x} + \pi_2 \int_{R_1} f_2(\mathbf{x}) \, \mathrm{d}\mathbf{x}$$

We want to find R_1 and R_2 so that this quantity is minimum. To find the solution we need to remember that

$$\begin{aligned} &\int_R f_1(\mathbf{x}) \, \mathrm{d}\mathbf{x} = 1, \\ &\int_R f_2(\mathbf{x}) \, \mathrm{d}\mathbf{x} = 1, \\ &R_1 \cup R_2 = R \\ &R_1 \cap R_2 = \emptyset \end{aligned}$$

Thus considering the first density can be split in the two areas

$$\int_R f_1(\mathbf{x}) \, \mathrm{d}\mathbf{x} = \int_{R_1} f_1(\mathbf{x}) \, \mathrm{d}\mathbf{x} + \int_{R_2} f_1(\mathbf{x}) \, \mathrm{d}\mathbf{x} = 1$$

So the quantity i'm interested in (the probability of wrong Π_2 classification of units belonging to Π_1) is

$$\int_{R_2} f_1(\mathbf{x}) \, \mathrm{d}\mathbf{x} = 1 - \int_{R_1} f_1(\mathbf{x}) \, \mathrm{d}\mathbf{x}$$

Going back to the total probability of wrong classification we have:

$$\begin{aligned} p &= \pi_1 \int_{R_2} f_1(\mathbf{x})\,\mathrm{d}\mathbf{x} + \pi_2 \int_{R_1} f_2(\mathbf{x})\,\mathrm{d}\mathbf{x} \\ &= \pi_1 \left[1 - \int_{R_1} f_1(\mathbf{x})\,\mathrm{d}\mathbf{x}\right] + \pi_2 \int_{R_1} f_2(\mathbf{x})\,\mathrm{d}\mathbf{x} \\ &= \pi_1 - \pi_1 \int_{R_1} f_1(\mathbf{x})\,\mathrm{d}\mathbf{x} + \pi_2 \int_{R_1} f_2(\mathbf{x})\,\mathrm{d}\mathbf{x} \\ &= \pi_1 + \int_{R_1} \pi_2 f_2(\mathbf{x}) - \pi_1 f_1(\mathbf{x})\,\mathrm{d}\mathbf{x} \end{aligned}$$

To minimize this, we have to chose R_1 such that the integral is minimum. And this occurs for values of $\mathbf{x}$ for which the integrand is negative

$$\begin{aligned} R_1 &= \{x : \pi_2 f_2(\mathbf{x}) - \pi_1 f_1(\mathbf{x}) < 0\} \\ &= \{x : \pi_1 f_1(\mathbf{x}) > \pi_2 f_2(\mathbf{x})\} \\ &= \left\{x : \frac{f_1(\mathbf{x})}{f_2(\mathbf{x})} > \frac{\pi_2}{\pi_1}\right\} \end{aligned}$$

In the last one the first inequality member is a likelihood ratio as seen before and the second the switched ratio on priors probability.
So similarly to what seen before the allocation rule will become

$$\begin{aligned} \frac{f_1(\mathbf{x}_0)}{f_2(\mathbf{x}_0)} > \frac{\pi_2}{\pi_1} &\implies \mathbf{x}_0 \in \Pi_1 \\ \frac{f_1(\mathbf{x}_0)}{f_2(\mathbf{x}_0)} < \frac{\pi_2}{\pi_1} &\implies \mathbf{x}_0 \in \Pi_2 \\ \frac{f_1(\mathbf{x}_0)}{f_2(\mathbf{x}_0)} > \frac{\pi_2}{\pi_1} &\implies \text{toss a coin to allocate} \end{aligned}$$

Important remark 44. This is the rule minimizing the total probability of a wrong classification in case of different prior probabilities: likelihood ratio are compared with inverse priors ratio. If $\pi_1 = \pi_2 = 1/2$, then the rule minimizing the total probability of a wrong classification coincides with the likelihood ratio rule seen before, otherwise results are different and take into account the fact theat different population have different prior probabilities.

Important remark 45. It is worth adding that the classification rule obtained by minimizing the total probability of a wrong classification is equivalent to the one that would be obtained by maximizing the posterior probability of population membership. That's the reason why it is often called an optimal Bayes rule.

5.2.3.3 Using Bayes Theorem

The same result above can be obtained using Bayes theorem. For the following:

- $\mathbb{P}(X \in \Pi_1 | X = \mathbf{x}_0)$ is the posterior probability for a observed unit to belong to population Π_1
- $\mathbb{P}(X = \mathbf{x}_0 | X \in \Pi_1) = f(X = \mathbf{x}_0 | X \in \Pi_1)$ is the likelihood of a single observation

we have that the posterior probability for population 1 and 2 can be rewritten according to Bayes rule as

$$\begin{aligned}
\mathbb{P}(X \in \Pi_1 | X = \mathbf{x}_0) &= \frac{\mathbb{P}(X \in \Pi_1) \cdot \mathbb{P}(X = \mathbf{x}_0 | X \in \Pi_1)}{\mathbb{P}(X \in \Pi_1) \cdot \mathbb{P}(X = \mathbf{x}_0 | X \in \Pi_1) + \mathbb{P}(X \in \Pi_2) \cdot \mathbb{P}(X = \mathbf{x}_0 | X \in \Pi_2)} \\
\mathbb{P}(X \in \Pi_2 | X = \mathbf{x}_0) &= \frac{\mathbb{P}(X \in \Pi_2) \cdot \mathbb{P}(X = \mathbf{x}_0 | X \in \Pi_2)}{\mathbb{P}(X \in \Pi_1) \cdot \mathbb{P}(X = \mathbf{x}_0 | X \in \Pi_1) + \mathbb{P}(X \in \Pi_2) \cdot \mathbb{P}(X = \mathbf{x}_0 | X \in \Pi_2)} \\
&= 1 - \mathbb{P}(X \in \Pi_1 | X = \mathbf{x}_0)
\end{aligned}$$

I can assign a unint to a population which have the largest posterior probability of coming from. The ensuing rule is called the optimal bayes's rule:

$$\begin{aligned}
&\frac{\mathbb{P}(X \in \Pi_1) \cdot \mathbb{P}(X = \mathbf{x}_0 | X \in \Pi_1)}{\mathbb{P}(X \in \Pi_1) \cdot \mathbb{P}(X = \mathbf{x}_0 | X \in \Pi_1) + \mathbb{P}(X \in \Pi_2) \cdot \mathbb{P}(X = \mathbf{x}_0 | X \in \Pi_2)} > \dots \\
&\dots \frac{\mathbb{P}(X \in \Pi_2) \cdot \mathbb{P}(X = \mathbf{x}_0 | X \in \Pi_2)}{\mathbb{P}(X \in \Pi_1) \cdot \mathbb{P}(X = \mathbf{x}_0 | X \in \Pi_1) + \mathbb{P}(X \in \Pi_2) \cdot \mathbb{P}(X = \mathbf{x}_0 | X \in \Pi_2)}
\end{aligned}$$

To simplify notation substitute the priors, eg $\mathbb{P}(X \in \Pi_1)$ with π_1 and likelihoods, eg $\mathbb{P}(X = \mathbf{x}_0 | X \in \Pi_2)$ with $f_2(\mathbf{x}_0)$. The rule becomes:

$$\begin{aligned}
&\frac{\pi_1 f_1(\mathbf{x}_0)}{\pi_1 f_1(\mathbf{x}_0) + \pi_2 f_2(\mathbf{x}_0)} > \frac{\pi_2 f_2(\mathbf{x}_0)}{\pi_1 f_1(\mathbf{x}_0) + \pi_2 f_2(\mathbf{x}_0)} \\
&\pi_1 f_1(\mathbf{x}_0) > \pi_2 f_2(\mathbf{x}_0) \\
&\frac{f_1(\mathbf{x}_0)}{f_2(\mathbf{x}_0)} > \frac{\pi_2}{\pi_1}
\end{aligned}$$

which ends to be the same rule found before: if above holds we assign to Π_1 otherwise to Π_2. The classification rule minimizing the total probability of a wrong classification is the optimal Bayes rule, that is, it assign a unit to the population it has the largest posterior probability of coming from

$$\begin{aligned}
R_1 &= \left\{ x : \frac{f_1(\mathbf{x}_0)}{f_2(\mathbf{x}_0)} > \frac{\pi_2}{\pi_1} \right\} \\
R_2 &= \left\{ x : \frac{f_1(\mathbf{x}_0)}{f_2(\mathbf{x}_0)} < \frac{\pi_2}{\pi_1} \right\}
\end{aligned}$$

this is the rule that we will use most of the cases.

5.2.3.4 Obtaining the likelihoods

Now the problem is still we said nothing on how to obtain the multivariate likelihoods (f_1 and f_2) for the last two coinciding rules (likelihood ratio and bayesian).

One way to do it is to define a model for $f_1(\mathbf{x})$ and $f_2(\mathbf{x})$ and then need to estimate the parameters. If $f_1(\mathbf{x})$ and $f_2(\mathbf{x})$ are multivariate normal distributions we have that the densities (il valore assoluto per indicare il determinante)

$$\begin{aligned}
f_1(\mathbf{x}) &= (2\pi)^{-p/2} |\mathbf{\Sigma}_1|^{-1/2} \exp\left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_1)^\top \mathbf{\Sigma}_1^{-1} (\mathbf{x} - \boldsymbol{\mu}_1) \right\} \\
f_2(\mathbf{x}) &= (2\pi)^{-p/2} |\mathbf{\Sigma}_2|^{-1/2} \exp\left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_2)^\top \mathbf{\Sigma}_2^{-1} (\mathbf{x} - \boldsymbol{\mu}_2) \right\}
\end{aligned}$$

Then the likelihoods ratio becomes

$$\frac{f_1(\mathbf{x})}{f_2(\mathbf{x})} = \ldots = |\boldsymbol{\Sigma}_1|^{-1/2} |\boldsymbol{\Sigma}_2|^{-1/2} \cdot \ldots$$
$$\ldots \cdot \exp\left\{ -\frac{1}{2} \left[\mathbf{x}^\top (\boldsymbol{\Sigma}_1 - \boldsymbol{\Sigma}_2)\mathbf{x} - 2\mathbf{x}^\top (\boldsymbol{\Sigma}_1^{-1}\boldsymbol{\mu}_1 - \boldsymbol{\Sigma}_2^{-1}\boldsymbol{\mu}_2) + \boldsymbol{\mu}_1^\top \boldsymbol{\Sigma}_1^{-1}\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2 \boldsymbol{\Sigma}_2^{-1}\boldsymbol{\mu}_2 \right] \right\}$$

People usually log this stuff above, obtaining

$$\begin{aligned}\log\left(\frac{f_1(\mathbf{x})}{f_2(\mathbf{x})}\right) &= \frac{1}{2}\log\left(\frac{|\boldsymbol{\Sigma}_2|}{|\boldsymbol{\Sigma}_1|}\right)\ldots \\ &- \frac{1}{2}\left[\mathbf{x}^\top (\boldsymbol{\Sigma}_1^{-1} - \boldsymbol{\Sigma}_2^{-1})\mathbf{x} - 2\mathbf{x}^\top (\boldsymbol{\Sigma}_1^{-1}\boldsymbol{\mu}_1 - \boldsymbol{\Sigma}_2^{-1}\boldsymbol{\mu}_2) + \boldsymbol{\mu}_1^\top \boldsymbol{\Sigma}_1^{-1}\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2^\top \boldsymbol{\Sigma}_2^{-1}\boldsymbol{\mu}_2 \right] \\ &= Q(\mathbf{x})\end{aligned}$$

$Q(\mathbf{x})$ is so called quadratic discriminant, a function for heteroschedastic normal population; with two mnv with different variances, the optimal surface that separate them is a quadratic surface (a parabola).
We need to compare $Q(\mathbf{x})$ with

- 0 (log of 1 where the two f are equivalent)
- $\log(\pi_2/\pi_1)$ if using populations with different prior

In case of homoscedasticity $\boldsymbol{\Sigma}_1 = \boldsymbol{\Sigma}_2 = \boldsymbol{\Sigma}$ the likelihood ratio simplifies

$$\begin{aligned}\frac{f_1(\mathbf{x})}{f_2(\mathbf{x})} &= |\boldsymbol{\Sigma}|^{-1/2} |\boldsymbol{\Sigma}|^{1/2} \cdot \exp\left\{ -\frac{1}{2} \left[\mathbf{x}^\top (\boldsymbol{\Sigma} - \boldsymbol{\Sigma})\mathbf{x} - 2\mathbf{x}^\top (\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1 - \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_2) + \boldsymbol{\mu}_1^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_2 \right] \right\} \\ &= \exp\left\{ -\frac{1}{2} \left[-2\mathbf{x}^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) + (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) \right] \right\} \\ &= \exp\left[\mathbf{x}^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) - \frac{1}{2}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) \right]\end{aligned}$$

Taking the log we obtain

$$\begin{aligned}\log\left(\frac{f_1(\mathbf{x})}{f_2(\mathbf{x})}\right) &= \mathbf{x}^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) - \frac{1}{2}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) \\ &\overset{(1)}{=} (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^\top \boldsymbol{\Sigma}^{-1}\mathbf{x} - \frac{1}{2}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)\end{aligned}$$

where in (1) is a scalar so i can transpose it obtaining the same. The final equation has to be compared to 0 or $\log(\pi_2/\pi_1)$ as usual.

This above is at the population level. At the sample level we estimate $\boldsymbol{\mu}_1$ with $\overline{\mathbf{x}}_1$ and $\boldsymbol{\mu}_2$ with $\overline{\mathbf{x}}_2$ and $\boldsymbol{\Sigma}$ with $\mathbf{W}$ and considering obtaining equal priors probability (thus comparing to 0) we have:

$$(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)^\top \mathbf{W}^{-1}\mathbf{x} > \frac{1}{2}(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)^\top \mathbf{W}^{-1}(\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)$$

Important remark 46. In it the allocation rule obtained according to Fisher's approach can be eas- ily recognized. This means that, for Gaussian populations and equal priors, besides optimizing group separation, Fisher's rule also minimizes the proba- bility of a wrong classification.
In conclusion: in the equal priors case for normal omoschedastic populations, fishers rule is optimal bayes rule.

Important remark 47. Other than hypotizing a MVN distribution of X the f density can be estimated in many different way: a simple way is to use naive bayes.

5.3 Lab

We seen different dataset where we know the groups.

5.3.1 Jobs

A large international air carrier has collected data on employees in three different job classifications:

1. customer service personnel
2. mechanics
3. dispatchers

The director of Human Resources wants to know if these three job classifications appeal to different personality types. Each employee is administered a battery of psychological tests which includes measures of interest in outdoor activity, sociability and conservativeness.

```
jobs <- read.csv("data/jobs.csv", header = TRUE, sep = ";")
head(jobs)

##   outdoor social conservative job
## 1      10     22            5   1
## 2      14     17            6   1
## 3      19     33            7   1
## 4      14     29           12   1
## 5      14     25            7   1
## 6      20     25           12   1

jobs$job <- factor(jobs$job,
                   levels = 1:3,
                   labels = c("Customer service",
                              "Mechanic",
                              "Dispatcher"))
```

The maximum number of useful discriminant functions that can separate the three jobs is less or equal to the minimum between $G-1$ and p, and so in this case it is less or equal to the minimum between 2 and 3, which is 2.
Thus, here we can find at most 2 useful discriminant functions to separate the employees by their jobs, using the 3 observed variables; these functions are the eigenvectors of $\mathbf{W}^{-1}\mathbf{B}$ which correspond to the not null eigenvalues.

```
## Some info on dimensions
p <- ncol(jobs) - 1
G <- length(unique(jobs$job))
n_tot <- nrow(jobs)   # total number of observation in all the two groups
```

Now we build the sub-datasets: dataset with only employees with each type

```
# we don't want the classification variables here for simplicity
jobs_split <- split(jobs[, -4], jobs$job)
lapply(jobs_split, head, n=2)

## $`Customer service`
##   outdoor social conservative
## 1      10     22            5
## 2      14     17            6
##
## $Mechanic
##    outdoor social conservative
## 86      20     27            6
## 87      21     15           10
##
## $Dispatcher
##     outdoor social conservative
## 179      19     19           16
## 180      17     17           12

n_g <- lapply(jobs_split, nrow)
```

5.3.1.1 Using standard matrix functions

To compute $W^{-1}B$ need to compute within and between group covariance matrix

Withing-group covariance matrix Defined as

$$W = \frac{1}{n-G}\sum_{g=1}^{G} S_g(n_g-1)$$

we start by calculating the covariance matrix of each group

```
Sg <- lapply(jobs_split, var) # covariance matrix within each group

W <- Reduce(function(x, y) x + y,
            Map(function(S, n) {S * (n - 1)},
                Sg, n_g)) /
  (n_tot - G)
```

Between-group covariance matrix Defined as

$$\mathbf{B} = \sum_{g=1}^{G} n_g(\overline{\mathbf{x}}_g - \overline{\mathbf{x}})(\overline{\mathbf{x}}_g - \overline{\mathbf{x}})^\top$$

```
xbarg <- lapply(jobs_split, colMeans) # average of variable in g-th group
xbar <- colMeans(jobs[, -4]) # overall average

B <- Reduce(function(x, y) x + y,
            Map(function(xb, n) { n * (xb - xbar) %*% t(xb - xbar)},
                xbarg, n_g)) /
  (G - 1)
```

Now, we are able to compute $\mathbf{W}^{-1}\mathbf{B}$ and, more specifically, we can define the (two) discriminant directions through its spectral decomposition.

Discriminant analysis via spectral decomposition Now we do SVD of $W^{-1}B$: we use `eigen`

```
spectral <- eigen(solve(W) %*% B)
round(spectral$values, 2)

## [1] 130.20  38.62   0.00
```

Only the first two are different from zero: this was expected: the maximum number of discriminant functions was 2.
Since we need to separate 3 groups on which 3 variables have been observed, the rank of the matrix $\mathbf{W}^{-1}\mathbf{B}$ is at most equal to 2; in fact there are two not null eigenvalues and two corresponding eigenvectors which are the discriminant coordinates or canonical variables.

Now we extract the canonical variables: the eigenvectors corresponding to not null eigenvalue

```
(A <- spectral$vectors[, 1:2])

##            [,1]       [,2]
## [1,]  0.3470958 -0.9130164
## [2,] -0.7331079 -0.2019912
## [3,]  0.5848738  0.3544018

colnames(jobs[, -4])

## [1] "outdoor"      "social"       "conservative"
```

A is 3×2 with in rows we have `outdoor`, `social` and `conservative`, while in column the coefficient obtained

Interpretation:

1. look at the coefficiente: the first function has a positive value for first and third, while negative for social. The first discriminant direction is a

linear contrast between interest in social activity and interest in outdoor or conservative activities. This means that the 3 employee categories mainly differ as far as the social component is concerned.

2. the second function has high negative value for outdoor, then a less negative for social and finaly a positive for conservative activities: seems a linear constrast of outtoor vs conservative activity.
   On the second discriminant direction outdoor activities and conservative activities have the largest effect. This direction separates employee categories according to the employees' attitudes towards static activities rather than more dynamic ones.

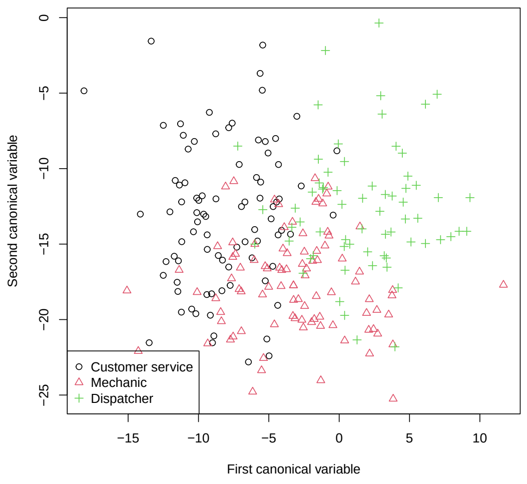
The discriminant directions are unique up to a change of sign. In particular, the sign depends on the normalization constraint imposed by the function used. Namely, eigenvectors obtained through the `eigen` function have unit norm; vectors provided by the `lda` (i.e. a function that will be described in the following) are computed by imposing that the within group covariance matrix is spherical.

Linear combinations Similarly to PC we can find linear comb between our data and the iscriminant function (project original data); we need just to transform our data in matrix

```r
X <- as.matrix(jobs[, -4])
Y <- X %*% A # linear combination
```

Thus, each unit is represented by a d-dimensional vector (where $d = rank(W^{-1}B)$). We can plot the obtained linear combinations

```r
plot(Y,
     xlab = "First canonical variable",
     ylab = "Second canonical variable",
     col = as.integer(jobs$job),
     pch = as.integer(jobs$job))

legend('bottomleft',
       legend = levels(jobs$job),
       col = 1:3,
       pch = 1:3)
```



These three groups seems not to be very separated according to first two canonical variables

5.3.1.2 Classification based on LDA

Now assume we need to assign a new observation (of unknown group) to one of the three profession.
We compare the distance of each observation to the average of the group, and then assign the observation to the group it is closer to. We can use the euclidean distance on the derived subspace or mahalanobis on the original subspace.

Euclidean distance between new points and the mean vector of the canonical variables First we need to project the average of the group in the derived/discriminant subspaces, that is we need to have $\overline{y}_1, \ldots \overline{y}_G$

```
(ybarg <- lapply(xbarg, function(x) x %*% A))

## $`Customer service`
##           [,1]      [,2]
## [1,] -8.136013 -13.1238
##
## $Mechanic
##           [,1]       [,2]
## [1,] -3.132914 -17.60166
##
## $Dispatcher
##          [,1]      [,2]
## [1,] 1.821577 -12.64947
```

The following code returns a matrix containing the Euclidean distances between each projected point from the projected means. We need to calculate the distance from every group, then we will assign to the closest one (this is just for didactical purposes)

```
## we build a martrix empty at the beginning
euclideanD <- matrix(NA, nrow = n_tot, ncol = G + 1)
# eg in 1,2 the distance between first obs and second group.
for (g in 1:G){
  # the g-th column contains the distance of every row with the g-th group
  euclideanD[, g] <- apply(Y,
                           1,
                           function(y){sqrt(sum((y - ybarg[[g]])^2))})
}

# for each row the observation and in each column the group
# in the last column we put the assigned group (1, 2 or 3)
euclideanD[, G+1] <- apply(euclideanD[, 1:G], 1, which.min)
head(euclideanD) # the last columns has the assigment

##          [,1]      [,2]      [,3] [,4]
## [1,] 2.073109  8.786252 11.585664    1
## [2,] 4.155567  3.641184  6.088613    2
## [3,] 9.975598 11.090576 17.713411    1
## [4,] 1.774625  7.027652 11.337834    1
## [5,] 2.548430  6.634660 11.517190    1
## [6,] 7.029186  1.908548  8.908554    2
```

Otherwise we can work on the original observations using the Mahalanobis distance.

Mahalanobis distance between each point and the mean vector of each group Working with

$$d_M^2(x_0, \overline{x}_g) = (x_0 - \overline{x}_g)^T W^{-1}(x_0 - \overline{x}_g)$$

Now we do the same with malahanobis distance but on the original variable

```
## structure is the same of the euclidean, we work on X instead
mahalanobisD <- matrix(NA, nrow = n_tot, ncol = G+1)
for (g in 1:G){
  # the g-th column contains the distance of every row with the g-th group
  # we work with X instead of Y
  mahalanobisD[, g] <- apply(
    X,
    1,
    function(x) t(x - xbarg[[g]]) %*% solve(W) %*% (x - xbarg[[g]])  # check
  )
}
mahalanobisD[, G+1] <- apply(mahalanobisD[, 1:G], 1, which.min)
head(mahalanobisD) # the last columns has the assigment

##           [,1]     [,2]      [,3] [,4]
## [1,] 1.9551699 6.772098 11.089305    1
## [2,] 3.7381503 3.348347  5.117959    2
## [3,] 6.8131739 8.986827 21.781321    1
## [4,] 1.9842879 5.148524 10.776851    1
## [5,] 0.5443612 3.178535  9.381197    1
## [6,] 4.0391721 1.139074  6.087088    2
```

Classification rule/missclassification rate In order to check the goodness of our classification and find the misclassification error (i.e. the proportion of observations not correctly assigned) we can compute a cross-table:

```
## elements on the main diagonal indicates units correctly classified
table(jobs$job, mahalanobisD[, 4])

##
##                       1  2  3
##   Customer service 70 11  4
##   Mechanic         16 62 15
##   Dispatcher        3 12 51
```

We can calculate

```
## missclassification rates
mean(as.integer(jobs$job) != mahalanobisD[, 4])

## [1] 0.25

## 25% of obs is wrongly classified
```

5.3.1.3 Using `MASS::lda`

Until here all done manually; to perform the analysis using functions, we can use `MASS::lda` which requires

- `x`: a matrix or data frame or Matrix containing the explanatory variables;
- `grouping`: a factor specifying the true class membership for each observation.

```
(lda_out <- MASS::lda(x = jobs[, -4], grouping = jobs$job))

## Call:
## lda(jobs[, -4], grouping = jobs$job)
##
## Prior probabilities of groups:
## Customer service         Mechanic       Dispatcher
##        0.3483607        0.3811475        0.2704918
##
## Group means:
##                      outdoor   social conservative
## Customer service 12.51765 24.22353     9.023529
## Mechanic         18.53763 21.13978    10.139785
## Dispatcher       15.57576 15.45455    13.242424
##
## Coefficients of linear discriminants:
##                      LD1         LD2
## outdoor       0.09198065 -0.22501431
## social       -0.19427415 -0.04978105
## conservative  0.15499199  0.08734288
##
## Proportion of trace:
##    LD1    LD2
## 0.7712 0.2288

A # for comparison

##             [,1]       [,2]
## [1,]  0.3470958 -0.9130164
## [2,] -0.7331079 -0.2019912
## [3,]  0.5848738  0.3544018
```

Coefficients of linear discriminants is what we called `A`. Discriminant function should be equivalent up to sign changes: however here results are different from what obtained with single value decomposition of $\mathbf{W}^{-1}\mathbf{B}$: `lda` uses a different constraint put on the within group covariance matrix, set to spherical.
That is usually we have

$$\mathbf{A}^{\top}\mathbf{W}\mathbf{A} = \mathbf{\Psi}$$

while results from `lda` are given for a A^* such that

$$\mathbf{A}^{*\top}\mathbf{W}\mathbf{A}^* = \mathbf{I}_{G-1}$$
$$\mathbf{A}^* = \mathbf{A}\mathbf{\Psi}^{-1/2}$$

if we want to obtain the same results as lda we need to compute this. To check, for Ψ

```
Psi = t(A) %*% W %*% A  #diagonal matrix (out of are almost zero)
Psi = diag(diag(Psi)) ## to have perfect diag
```

then multiplying A vectors for $\Psi^{-1/2}$ we find again the coefficients of the linear discriminants yield by `lda`

```
(Astar = A %*% solve(Psi^{1/2})) # vector of coefficients

##              [,1]        [,2]
## [1,]  0.09198065 -0.22501431
## [2,] -0.19427415 -0.04978105
## [3,]  0.15499199  0.08734288

lda_out$scaling # the same
```

```
##                       LD1         LD2
## outdoor       0.09198065 -0.22501431
## social       -0.19427415 -0.04978105
## conservative  0.15499199  0.08734288
```

if we use Astar instead of A we get identity

```
t(Astar) %*% W %*% Astar

##               [,1]          [,2]
## [1,]  1.000000e+00 -6.106227e-16
## [2,] -6.938894e-16  1.000000e+00
```

And the opposite is true, i.e. if we divide the coefficients of the linear discriminants yield by lda by $\Psi^{-1/2}$ we obtain the solution given by the eigen function:

```
coef(lda_out) %*% solve(solve(Psi)^(1/2))

##                    [,1]       [,2]
## outdoor       0.3470958 -0.9130164
## social       -0.7331079 -0.2019912
## conservative  0.5848738  0.3544018
```

Note: this equivalence holds as far as the conventional definition of matrix B is considered, i.e. groups are weighted by their size in the dataset. The lda function also allows to consider a covariance matrix weighted by the prior probabilities of the classes if these are specified; otherwise observed frequencies are used.

Canonical variates with lda We use `predict` to obtain the projection on the unidimensional space

```
pred <- predict(lda_out) # class, prediction ,posterior is the posterior prob
# matrix and x is the projected units

Ylda <- pred$x
head(Ylda) # should be equal

##             LD1         LD2
## [1,] -1.6423155  0.71477348
## [2,] -0.1480302  0.15096436
## [3,] -2.6415213 -1.68326115
## [4,] -1.5493681  0.07764901
## [5,] -1.5472314 -0.15994117
## [6,] -0.2203876 -1.07331266

head(Y) # very different

##             [,1]      [,2]
## [1,]  -9.733047 -11.80196
## [2,]  -4.094251 -14.08967
## [3,] -13.503624 -21.53221
## [4,]  -9.382303 -14.38715
## [5,]  -9.374240 -15.35120
## [6,]  -4.367296 -19.05729
```

They are different because use Astar instad of A. also if we try to use Astar does not work because data is centered by lda. So we need to center X to obtain the same results

```
head(scale(X, center = TRUE, scale = FALSE) %*% Astar) # same results

##             [,1]        [,2]
## [1,] -1.6423155  0.71477348
## [2,] -0.1480302  0.15096436
## [3,] -2.6415213 -1.68326115
## [4,] -1.5493681  0.07764901
## [5,] -1.5472314 -0.15994117
## [6,] -0.2203876 -1.07331266
```

5.3.2 Banknotes

A manager of a bank want to discriminate between genuine and counterfeit banknotes. The following dataset include measures of 100 genuine and 100 false/counterfeit banknotes

```
head(banknotes <- read.csv("data/banknotes.csv", sep = ";"))

##   Length  Left Right Bottom  Top Diagonal
## 1  214.8 131.0 131.1    9.0  9.7    141.0
## 2  214.6 129.7 129.7    8.1  9.5    141.7
## 3  214.8 129.7 129.7    8.7  9.6    142.2
## 4  214.8 129.7 129.6    7.5 10.4    142.0
## 5  215.0 129.6 129.7   10.4  7.7    141.8
## 6  215.7 130.8 130.5    9.0 10.1    141.4

## first 100 are true/genuine, last 100 are false
group <- c(rep("Genuine", 100), rep("Counterfeit", 100))
```

We want to separate $G = 2$ groups in which $p = 5$ variables have been observed. The rank of matrix $\mathbf{W}^{-1}\mathbf{B}$ is thus equal to 1. This means that there is only one not null eigenvalue; the corresponding eigenvector is the only discriminant coordinate (or canonical variable)

```
(lda_out <- MASS::lda(x=banknotes, grouping = group)) # only 1 discriminant function

## Call:
## lda(banknotes, grouping = group)
```

```
##
## Prior probabilities of groups:
## Counterfeit     Genuine
##         0.5         0.5
##
## Group means:
##              Length    Left   Right Bottom    Top Diagonal
## Counterfeit 214.823 130.300 130.193 10.530 11.133  139.450
## Genuine     214.969 129.943 129.720  8.305 10.168  141.517
##
## Coefficients of linear discriminants:
##                   LD1
## Length    0.005011113
## Left      0.832432523
## Right    -0.848993093
## Bottom   -1.117335597
## Top      -1.178884468
## Diagonal  1.556520967
```

We have positive value for left and diagonal and negative for other. The discriminant direction is a linear contrast between the length of the diagonal and the length of the left rim versus height of the right, bottom and top rims. This means that genuine and counterfeit banknotes mainly differ for the length of the diagonal (which summarizes the total dimensions of the notes) and for the length of the left rim with respect to all the other ones.

The linear combination is then $\mathbf{Y} = \mathbf{XA}$ where X is the $n \times p$ data matrix and $\mathbf{A}$ is the $p \times 1$ matrix whose columns are the eigenvectors of $\mathbf{W}^{-1}\mathbf{B}$ corresponding to the non null eigenvalues. Thus, each unit is represented by a one-dimensional vector.

Performing classification Classification can be performed using the predict function. This function classifies multivariate observations by projecting them onto the linear discriminant direction(s) found by lda. It takes as first argument the output of the model fitting and as second one the set of units whose membership has to be predicted. If the latter is equal to the set of units used to fit the model, it can be omitted. The output provides:

- `class`: predicted class membership of each observation;
- `posterior`: posterior probabilities for the classes;
- `x`: scores (observations on the discriminant directions).

```
pred <- predict(lda_out)
```

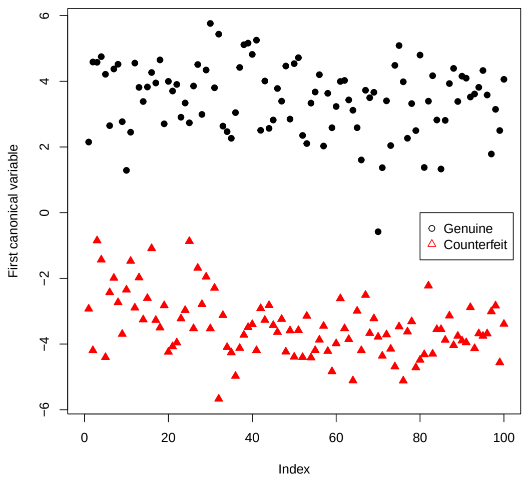
Now we can tabulate the obtained classifications with the true ones:

```
table(group, pred$class) # almost perfect (only 1 banknotes misclassified)
```

```
##
## group          Counterfeit Genuine
##    Counterfeit         100       0
##    Genuine               1      99
```

The classification is almost perfect: only one unit is misclassified probably because it presents an irregular shape close to the original one.
The plot of the units projected onto the space spanned by the canonical variable is obtained as it follows. Banknotes are coloured by the group membership.

```
Y <- pred$x # one dimensional projections
# plot(Y) # not what we want the index separates the groups

# plot all in the 1:100 xlim of index
plot(Y, type = "n", xlim = c(0, 100), # don't plot anything but setup
     ylab = "First canonical variable")
points(Y[1:100], pch = 21, col = "black", bg = "black")
points(Y[101:200], pch = 24, col = "red", bg = "red")
legend(80, 0, c("Genuine", "Counterfeit"),
       col = c("black", "red"), pch = c(21, 24))
```



5.3.3 Wisconsin Diagnostic Breast Cancer (WDBC) Data

This data comes from UCI Machine Learning Repository. It contains 30 regressors, physical measurements of cancer cells, and a binary response containing the diagnosis M (malignant) or B (benign).
We will apply a classifier based on linear discriminant analysis, but we will try to assess its performance by splitting the data in two subsets: a training set and a test set. Indeed, in statistics, goodness of fit refers to how closely a model's predicted values match the observed (true) values. In order to prevent a phenomenon called overfitting (i.e. the production of an analysis that corresponds

too closely or exactly to a particular set of data), it is common to partition the available data in two separate parts. One of them, called training set, is used to estimate the model's parameters, whereas the other, called test set, is employed to validate them.

```
head(wdbc <- read.csv("data/wdbc.csv"))

##   response    V3    V4     V5     V6      V7      V8     V9     V10    V11
## 1        M 17.99 10.38 122.80 1001.0 0.11840 0.27760 0.3001 0.14710 0.2419
## 2        M 20.57 17.77 132.90 1326.0 0.08474 0.07864 0.0869 0.07017 0.1812
## 3        M 19.69 21.25 130.00 1203.0 0.10960 0.15990 0.1974 0.12790 0.2069
## 4        M 11.42 20.38  77.58  386.1 0.14250 0.28390 0.2414 0.10520 0.2597
## 5        M 20.29 14.34 135.10 1297.0 0.10030 0.13280 0.1980 0.10430 0.1809
## 6        M 12.45 15.70  82.57  477.1 0.12780 0.17000 0.1578 0.08089 0.2087
##       V12    V13    V14   V15    V16      V17     V18     V19     V20     V21
## 1 0.07871 1.0950 0.9053 8.589 153.40 0.006399 0.04904 0.05373 0.01587 0.03003
## 2 0.05667 0.5435 0.7339 3.398  74.08 0.005225 0.01308 0.01860 0.01340 0.01389
## 3 0.05999 0.7456 0.7869 4.585  94.03 0.006150 0.04006 0.03832 0.02058 0.02250
## 4 0.09744 0.4956 1.1560 3.445  27.23 0.009110 0.07458 0.05661 0.01867 0.05963
## 5 0.05883 0.7572 0.7813 5.438  94.44 0.011490 0.02461 0.05688 0.01885 0.01756
## 6 0.07613 0.3345 0.8902 2.217  27.19 0.007510 0.03345 0.03672 0.01137 0.02165
##        V22   V23   V24    V25    V26    V27    V28    V29    V30    V31     V32
## 1 0.006193 25.38 17.33 184.60 2019.0 0.1622 0.6656 0.7119 0.2654 0.4601 0.11890
## 2 0.003532 24.99 23.41 158.80 1956.0 0.1238 0.1866 0.2416 0.1860 0.2750 0.08902
## 3 0.004571 23.57 25.53 152.50 1709.0 0.1444 0.4245 0.4504 0.2430 0.3613 0.08758
## 4 0.009208 14.91 26.50  98.87  567.7 0.2098 0.8663 0.6869 0.2575 0.6638 0.17300
## 5 0.005115 22.54 16.67 152.20 1575.0 0.1374 0.2050 0.4000 0.1625 0.2364 0.07678
## 6 0.005082 15.47 23.75 103.40  741.6 0.1791 0.5249 0.5355 0.1741 0.3985 0.12440

## divide the dataset using sample
set.seed(19)
n <- nrow(wdbc)
train <- sample(n, size = n * 2/3, replace =FALSE) # 2/3 to train  1/3 to test

wdbc_train <- wdbc[train, ]
wdbc_test <- wdbc[-train, ]
```

Partitioning the dataset

```
lda_out <- MASS::lda(x = wdbc_train[, -1], grouping = wdbc_train[, 1])
```

Compute discriminant directions by lda Predictions for the training data and wrong missclassification in the training set

```
class_train <- predict(lda_out)$class
C <- table(class_train, wdbc_train[, 1])
1 - sum(diag(C)) / sum(C)

## [1] 0.02902375
```

Predictions for the test data and right missclassification in the test set (we see error is higher, but right, compared to previous one)

```
class_test <- predict(lda_out, newdata = wdbc_test[, -1])$class
C <- table(class_test, wdbc_test[, 1])
1 - sum(diag(C)) / sum(C)

## [1] 0.07894737
```