Statistics for the Sciences - Part 3

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November 7, 2023

Covariance and correlation matrices

Covariance and Correlation

The **covariance** of two random variables X and Y is

$$\sigma_{XY} = E[(X - \mu_X)(Y - \mu_Y)]$$

and their **correlation coefficient** is

$$\rho_{XY} = \frac{\sigma_{XY}}{\sigma_X \sigma_Y}$$

Covariance and Correlation - sample

Given a sample consisting of pairs $\{(x_i, y_i) : i = 1, \ldots, n\}$, the **Pearson's correlation coefficient** is

$$r_{xy} = \frac{s_{xy}}{s_x \, s_y}$$

where

$$\begin{aligned} s_{xy} &= \tfrac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}) \\ s_x^2 &= \tfrac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2 \\ s_y^2 &= \tfrac{1}{n-1}\sum_{i=1}^{n}(y_i - \bar{y})^2 \end{aligned}$$

Covariance and Correlation

For random variables X and Y, ρ_{XY} measures **linear dependence** between X and Y.
ρ_{XY} is bouded:

$$-1 \leq \rho_{XY} \leq 1$$

- $\rho_{XY} = -1$ implies perfect negative linear relationship
- $\rho_{XY} = 1$ implies perfect positive linear relationship
- $\rho_{XY} = 0$ implies no linear relationship

NOTE: Correlation does not implies causation, not independence ($\rho_{XY} = 0$ does not imply that X and Y are independent).

Covariance and Correlation

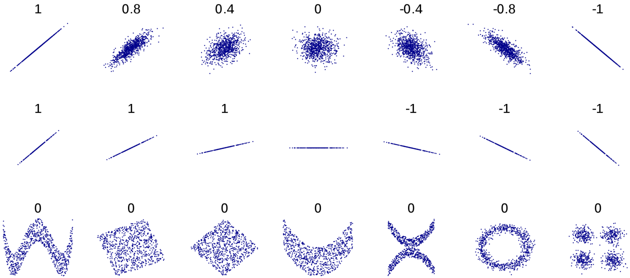
Property: ρ_{XY} is unaffected by linear transformations.

Suppose that $X^{'} = aX + b$ and $Y^{'} = cY + d$. Then

- $\rho_{X'Y'} = \rho_{XY} \quad$ if $\operatorname{sgn}(a) = \operatorname{sgn}(c)$
- $\rho_{X'Y'} = -\rho_{XY} \quad$ if $\operatorname{sgn}(a) \neq \operatorname{sgn}(c)$

This property can be proved directly using the definition of correlation.

Covariance and Correlation - sample



Several sets of points with the corresponding Pearson correlation coefficient r_{xy}.

- r_{xy} reflects noisiness and direction of linear relationship (top row)
- it does not measure the slope of the relationship (middle row)
- it does not capture many aspects of nonlinear relationships (bottom row)

Correlation - example

Example. The following survey reports several measurements collected by 5 instructors for students in their classes related to their nutrition education program. We want to explore the relationship between Sodium and Calories.

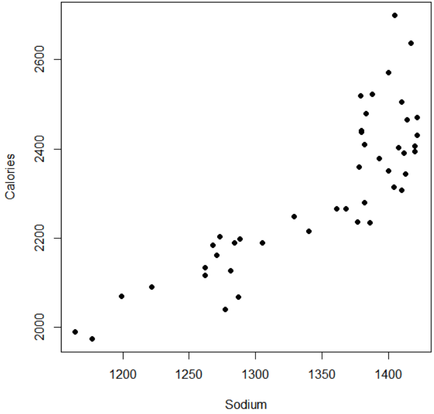
```
Data <- read.csv("C:/Users/student_survey.csv")
> head(Data)
```

	Instructor	*Grade*	*Weight*	*Calories*	*Sodium*	*Score*
1	*BrendonSmall*	6	43	2069	1287	77
2	*BrendonSmall*	6	41	1990	1164	76
3	*BrendonSmall*	6	40	1975	1177	76
4	*BrendonSmall*	6	44	2116	1262	84
5	*BrendonSmall*	6	45	2161	1271	86
6	*BrendonSmall*	6	44	2091	1222	87
...	...	...	...	...	...	...

Correlation - example

Here is the plot of the data showing the relationship between Calories (y) and Sodium (x).

```
> plot(Calories ~ Sodium,data=Data,pch=16,ylab =
"Calories", xlab = "Sodium")
```



Correlation - example

Compute correlation in R

Correlation coefficient can be computed using the functions `cor()` or `cor.test()`

- `cor()` computes the correlation coefficient
- `cor.test()` tests for association/correlation between paired samples. It returns both the correlation coefficient and the significance level (or p-value) of the correlation .

Commands formats are:

- `cor(x, y, method = c("pearson", "kendall", "spearman"))`
- `cor.test(x, y, method=c("pearson", "kendall", "spearman"))`

Correlation - example

The Pearson's correlation coefficient is a measure of linear association. The significance test works under the assumption that x and y are sampled from a bivariate normal distribution.

```
> cor(Data$Sodium,Data$Calories, method = "pearson")
[1] 0.8489548
```

The Kendall and Spearman correlation coefficients are **rank-based** measure of association. This may may be used if the data do not necessarily come from a bivariate normal distribution.

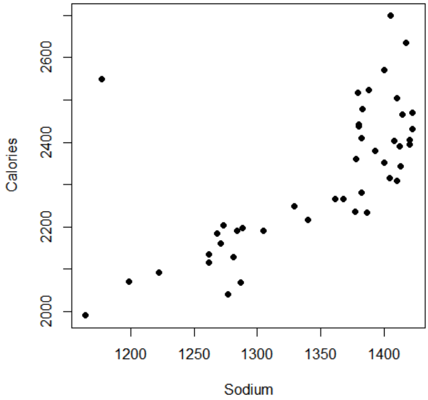
```
> cor(Data$Sodium,Data$Calories, method = "kendall")
[1] 0.6490902
```

```
> cor(Data$Sodium,Data$Calories, method = "spearman")
[1] 0.8201766
```

Correlation - example

Correlation is very sensitive to outliers.

Here we modify a single point in the dataset



Correlation - example

Here are the re-computed correlation coefficients; in parenthesis is the value we calculated above.

```
> cor(Data2$Sodium,Data$Calories, method = "pearson")
```

[1] 0.6866076 (0.8489548)

```
> cor(Data2$Sodium,Data$Calories, method = "kendall")
```

[1] 0.5699824 (0.6490902)

```
> cor(Data2$Sodium,Data$Calories, method =
"spearman")
```

[1] 0.7088825 (0.8201766)

Correlation - example

We want to test if there is a linear relationship between Calories (Y) and Sodium (X) at significance level $\alpha = 0.01$.

Hypothesis testing problem:

$$\begin{aligned} H_0 : &\quad \rho_{X,Y} = 0 \\ H_1 : &\quad \rho_{X,Y} \neq 0 \end{aligned}$$

<u>If (X, Y) follows a bivariate normal distribution</u> with $\rho_{X,Y} = 0$ and if the samples $\{(x_i, y_i) : i = 1, \dots n\}$ are i.i.d., then

$$T = \frac{r_{xy}\sqrt{n-2}}{\sqrt{1 - r_{xy}^2}} \sim t_{n-2}$$

Hence, we can reject H_0 if $|T| > t_{\alpha/2;n-2}$ where, as usual, $t_{\alpha/2;n-2}$ is the critical value of the t distribution such that $P(T \geq t_{\alpha/2;n-2}) > \alpha/2$.

Correlation - example

Under the assumption above, we can apply the Pearson's correlation analysis

```
> cor.test(Data$Sodium,Data$Calories, method = "pearson")
```

Pearson's product-moment correlation

data: Data$Sodium and Data$Calories

t = 10.534, df = 43, p-value = 1.737e-13

alternative hypothesis: true correlation is not equal to 0

95 percent confidence interval:

0.7397691 0.9145785

sample estimates:

cor

0.8489548

Since p-value = 1.737e-13, we reject the null hypothesis at significance level α = 0.01 (or any other value above the p-value) and accept the alternative hypothesis that $\rho_{X,Y} \neq 0$.

Correlation - example

If the assumption that data come from a normal distribution cannot be satisfied, we can apply the **Spearman's rho statistic** that estimates a rank-based measure of association.

```
> cor.test(Data$Sodium,Data$Calories, method = "spearman")
```

Spearman's rank correlation rho

data: Data$Sodium and Data$Calories
S = 2729.7, p-value = 5.443e-12
alternative hypothesis: true rho is not equal to 0
sample estimates:
rho
0.8201766

Since p-value = 5.443e-12, we reject the null hypothesis at significance level α = 0.01 (or any other value above the p-value) and accept the alternative hypothesis that $\rho_{X,Y} \neq 0$.

Non-parametric correlation

Spearman's rho statistic measures a **rank-based measure of association.**

This test may be used if the data do not come from a bivariate normal distribution. it only requires that each variable at least be measured on the ordinal scale.

Spearman's correlation determines the strength and direction of the **monotonic relationship** between your two variables rather than the strength and direction of the **linear relationship** between your two variables, which is what Pearson's correlation determines.

Monotonicity is less restrictive than a linear relationship.

A monotonic relationship is a relationship that does one of the following: (1) as the value of one variable increases, so does the value of the other variable; or (2) as the value of one variable increases, the other variable value decreases.

Correlation test

If we want to test the more general hypothesis testing problem

$$\begin{aligned} H_0 : &\quad \rho_{X,Y} = \rho_0 \\ H_1 : &\quad \rho_{X,Y} \neq \rho_0, \end{aligned}$$

with $\rho_0 \neq 0$, the mathematical setting becomes more complicated since - still under the assumption that (X, Y) follows a bivariate normal distribution and that the samples $\{(x_i, y_i) : i = 1, \dots n\}$ are i.i.d. - the formulation of the test statistic becomes more involved and can be solved using the Fisher's z-transformation.

Correlation test - example

Example: we test $H_0 : \rho_{X,Y} = 0.7$ vs $H_1 : \rho_{X,Y} \neq 0.7$, with

We define the `fisherz` function

```
> fisherz=function(r,n,rho0=0){
+ z=log((1+r)/(1-r))/2
+ z0=log((1+rho0)/(1-rho0))/2
+ zstar=(z-z0)*sqrt(n-3)
+ pval=2*(1-pnorm(abs(zstar)))
+ list(pval=pval)}
```

In our example, setting $n = 45$ and $\rho_0 = 0.7$, we compute

```
> fisherz(cor(Data$Sodium,Data$Calories),45,rho0=0.7)
```

\$pval = 0.01257023

Data matrix

In applications, it may be useful to compute correlations for several pairs of variables.

Suppose we have a $n \times p$ data matrix

$$X = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix}$$

- n items/subjects are listed as rows
- p variables are listed as columns

Example: mtcars (Motor Trend Car Road Tests)

The R data set `mtcars` was extracted from the 1974 Motor Trend magazine, and comprises fuel consumption and 10 aspects of car design and performance for 32 automobiles models from 1973-74.

Data frame consists of 32 observations on 11 variables.

[,1]	mpg	Miles/gallon
[,2]	cyl	Number of cylinders
[,3]	disp	Displacement (cu.in.)
[,4]	hp	Gross horsepower
[,5]	drat	Rear axle ratio
[,6]	wt	Weight (lbs/1000)
[,7]	qsec	1/4 mile time
[,8]	vs	Engine (0 = V-shaped, 1 = straight)
[,9]	am	Transmission (0 = automatic, 1 = manual)
[,10]	gear	Number of forward gears
[,11]	carb	Number of carburetors

Data matrix example - mtcars

We load the dataset. As remarked above, it consists of 32 observations of 11 variables.

```
> data(mtcars)
> dim(mtcars)
[1] 32 11
> head(mtcars)
```

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
MazdaRX4	21.0	6	160	110	3.90	2.620	16.46	0	1	4	4
MazdaRX4Wag	21.0	6	160	110	3.90	2.875	17.02	0	1	4	4
Datsun710	22.8	4	108	93	3.85	2.320	18.61	1	1	4	1
Hornet4Drive	21.4	6	258	110	3.08	3.215	19.44	1	0	3	1
HornetSportabout	18.7	8	360	175	3.15	3.440	17.02	0	0	3	2
Valiant	18.1	6	225	105	2.76	3.460	20.22	1	0	3	1

Data matrix example - mtcars

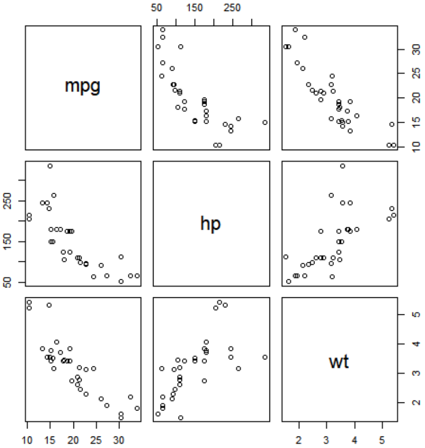
One can explore some statistical properties of the dataset using `summary(mtcars)`.

```
> summary(mtcars)
      mpg             cyl             disp             hp             drat
 Min.   :10.40   Min.   :4.000   Min.   : 71.1   Min.   : 52.0   Min.   :2.760
 1st Qu.:15.43   1st Qu.:4.000   1st Qu.:120.8   1st Qu.: 96.5   1st Qu.:3.080
 Median :19.20   Median :6.000   Median :196.3   Median :123.0   Median :3.695
 Mean   :20.09   Mean   :6.188   Mean   :230.7   Mean   :146.7   Mean   :3.597
 3rd Qu.:22.80   3rd Qu.:8.000   3rd Qu.:326.0   3rd Qu.:180.0   3rd Qu.:3.920
 Max.   :33.90   Max.   :8.000   Max.   :472.0   Max.   :335.0   Max.   :4.930
       wt             qsec             vs               am              gear
 Min.   :1.513   Min.   :14.50   Min.   :0.0000   Min.   :0.0000   Min.   :3.000
 1st Qu.:2.581   1st Qu.:16.89   1st Qu.:0.0000   1st Qu.:0.0000   1st Qu.:3.000
 Median :3.325   Median :17.71   Median :0.0000   Median :0.0000   Median :4.000
 Mean   :3.217   Mean   :17.85   Mean   :0.4375   Mean   :0.4062   Mean   :3.688
 3rd Qu.:3.610   3rd Qu.:18.90   3rd Qu.:1.0000   3rd Qu.:1.0000   3rd Qu.:4.000
 Max.   :5.424   Max.   :22.90   Max.   :1.0000   Max.   :1.0000   Max.   :5.000
      carb
 Min.   :1.000
 1st Qu.:2.000
 Median :2.000
 Mean   :2.812
 3rd Qu.:4.000
 Max.   :8.000
```

Data matrix example - mtcars

You can also visually explore the dataset by to visualizing the relationship for several pairs of variable

```
> pairs(mtcars[, c("mpg", "hp", "wt")])
```



Data matrix - example

We will use this example to illustrate how to work with a data matrix in R.

Computation of **column means** (first 3 columns)

```
> X <- as.matrix(mtcars)
> colMeans(X)[1:3]
```

mpg	*cyl*	*disp*
20.09062	6.18750	230.72188

This is an alternate way to carry out the same computation

```
> apply(X,2,mean)[1:3]
```

mpg	*cyl*	*disp*
20.09062	6.18750	230.72188

Data matrix - example

One can similarly compute other statistical functions.

Computation of **column median** (first 3 columns)

```
> apply(X,2,median)[1:3]
```

mpg	*cyl*	*disp*
19.2	6.0	196.3

Computation of **column range** (first 3 columns)

```
> apply(X,2,range)[,1:3]
```

	mpg	*cyl*	*disp*
[1,]	10.4	4	71.1
[2,]	33.9	8	472.0

Correlation matrix

Let X be a $n \times p$ data matrix, containing p vectors of length n ordered by columns.

The **correlation matrix** of X is the $p \times p$ symmetric matrix

$$R = \begin{pmatrix} 1 & r_{12} & \dots & r_{1p} \\ r_{21} & 1 & \dots & r_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ r_{p1} & r_{p2} & \dots & 1 \end{pmatrix}$$

where the entries are the pairwise correlations $r_{ij} = r_{ji} = \frac{s_{ij}}{s_i s_j}$ for $1 \leq i, j \leq p$ and $r_{ii} = 1$.

The matrix R contains all the pair-wise correlation coefficients between any column vectors in the matrix X.

Correlation matrix

We want to compute the correlation matrix of the `mtcars` matrix

We first remove the categorical variables `vs` and `am`.

```
library(tidyverse)
X <- mtcars %>% select(-vs, -am)
```

The new data matrix X has dimension 32×9

```
> dim(X)
```

[1] 32 9

```
> head(X)
```

	mpg	*cyl*	*disp*	*hp*	*drat*	*wt*	*qsec*	*gear*	*carb*
MazdaRX4	21.0	6	160	110	3.90	2.620	16.46	4	4
MazdaRX4Wag	21.0	6	160	110	3.90	2.875	17.02	4	4
Datsun710	22.8	4	108	93	3.85	2.320	18.61	4	1
Hornet4Drive	21.4	6	258	110	3.08	3.215	19.44	3	1
HornetSportabout	18.7	8	360	175	3.15	3.440	17.02	3	2
Valiant	18.1	6	225	105	2.76	3.460	20.22	3	1

Correlation matrix

We compute the correlation matrix of the modified `mtcars` matrix. For easier reading, correlation coefficients are rounded to 2 decimal digits.

```
> round(cor(X), digits = 2)
```

	mpg	cyl	disp	hp	drat	wt	qsec	gear	carb
mpg	1.00	−0.85	−0.85	−0.78	0.68	−0.87	0.42	0.48	−0.55
cyl	−0.85	1.00	0.90	0.83	−0.70	0.78	−0.59	−0.49	0.53
disp	−0.85	0.90	1.00	0.79	−0.71	0.89	−0.43	−0.56	0.39
hp	−0.78	0.83	0.79	1.00	−0.45	0.66	−0.71	−0.13	0.75
drat	0.68	−0.70	−0.71	−0.45	1.00	−0.71	0.09	0.70	−0.09
wt	−0.87	0.78	0.89	0.66	−0.71	1.00	−0.17	−0.58	0.43
qsec	0.42	−0.59	−0.43	−0.71	0.09	−0.17	1.00	−0.21	−0.66
gear	0.48	−0.49	−0.56	−0.13	0.70	−0.58	−0.21	1.00	0.27
carb	−0.55	0.53	0.39	0.75	−0.09	0.43	−0.66	0.27	1.00

The matrix is symmetric and has diagonal 1, as expected.
This correlation matrix gives an overview of the correlations for all combinations of two variables in X.

Note: we can compute in a very similar way the Spearman correlation matrix. The modified command is as follows:

```
> round(cor(X,method="spearman"), digits = 2 )
```

Correlation matrix

Interpretation of correlation matrix

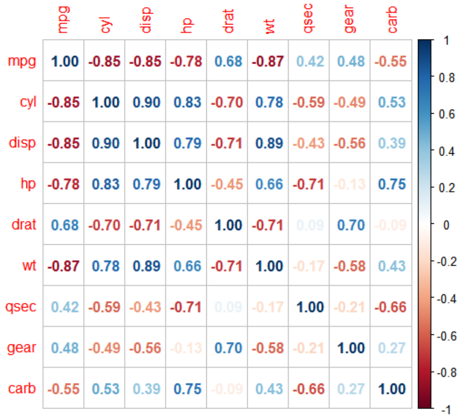
	mpg	*cyl*	*disp*	*hp*	*drat*	*wt*	*qsec*	*gear*	*carb*
mpg	1.00	−0.85	−0.85	−0.78	0.68	−0.87	0.42	0.48	−0.55
cyl	−0.85	1.00	0.90	0.83	−0.70	0.78	−0.59	−0.49	0.53
disp	−0.85	0.90	1.00	0.79	−0.71	0.89	−0.43	−0.56	0.39
hp	−0.78	0.83	0.79	1.00	−0.45	0.66	−0.71	−0.13	0.75
drat	0.68	−0.70	−0.71	−0.45	1.00	−0.71	0.09	0.70	−0.09
wt	−0.87	0.78	0.89	0.66	−0.71	1.00	−0.17	−0.58	0.43
qsec	0.42	−0.59	−0.43	−0.71	0.09	−0.17	1.00	−0.21	−0.66
gear	0.48	−0.49	−0.56	−0.13	0.70	−0.58	−0.21	1.00	0.27
carb	−0.55	0.53	0.39	0.75	−0.09	0.43	−0.66	0.27	1.00

The correlation between horsepower (hp) and miles per gallon (mpg) found above is -0.78, meaning that the 2 variables vary in opposite direction. This makes sense, cars with more horsepower tend to consume more fuel (and thus have a lower millage par gallon). On the contrary, from the correlation matrix we see that the correlation between miles per gallon (mpg) and the time to drive 1/4 of a mile (qsec) is 0.42, meaning that fast cars (low qsec) tend to have a worse millage per gallon (low mpg). This again make sense as fast cars tend to consume more fuel.

Correlation matrix

The R package `corrplot` provides a visual exploratory tool for the correlation matrix.

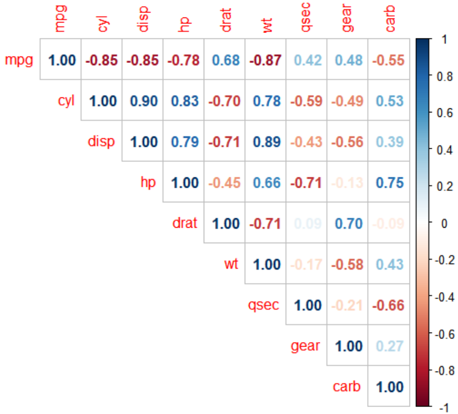
```
> library(corrplot)
> corrplot(cor(X),method = "number")
```



Correlation matrix

Since the matrix is symmetric, we only need to visualize the upper or lower half.

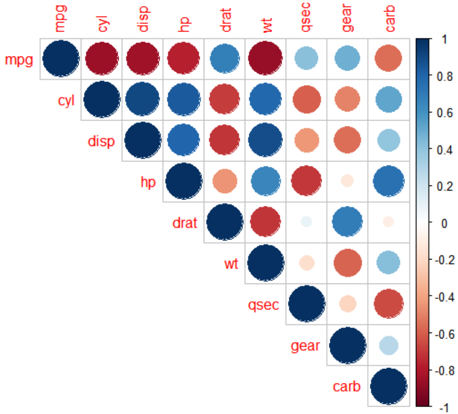
```
> corrplot(cor(X),method = "number",type = "upper")
```



Correlation matrix

Rather than displaying numerical values, one can use colors.

```
> corrplot(cor(X), method = "circle",type = "upper")
```



Correlation matrix

One important application of the correlation matrix is to investigate if there are patterns among specific groups of variables.

The package `corrplot` supports automatic variable reordering.

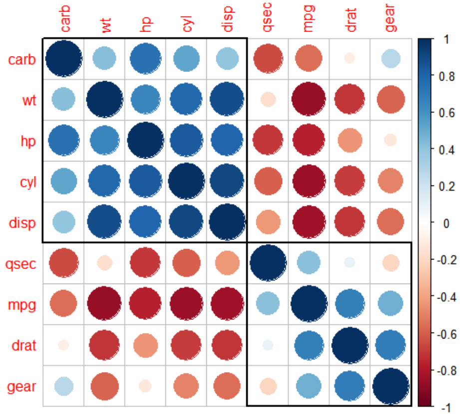
Four order algorithms are available: 'AOE', 'FPC', 'hclust', 'alphabet'.

- 'AOE' is for the angular order of the eigenvectors. It is calculated from the order of the angles corresponding to the largest two eigenvalues of the correlation matrix.
- 'FPC' for the first principal component order.
- 'hclust' for hierarchical clustering order, and 'hclust.method' for the agglomeration method to be used. 'hclust.method' should be one of 'ward', 'ward.D', 'ward.D2', 'single', 'complete', 'average', 'mcquitty', 'median' or 'centroid'.
- 'alphabet' for alphabetical order.

Correlation matrix

The option 'hclust' draws rectangles around the plot of correlation matrix based on the results of hierarchical clustering.

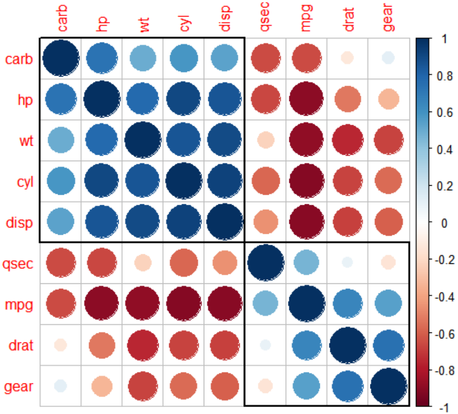
```
> corrplot(cor(X), order = 'hclust', addrect = 2)
```



Correlation matrix

Here we compute again the correlation matrix with the variables reordered based on the results of hierarchical clustering but we use the Spearman correlation.

```
> corrplot(cor(X,method="spearman"), order = 'hclust',
addrect = 2)
```



Correlation matrix

Similar to the `cor()` command used to compute correlation for several pairs of variables in a matrix, the `rcorr()` function from the `Hmisc` package is useful to analyze the correlation matrix.

```
rcorr(X, type=c("pearson","spearman"))
```

It returns

1. the correlation matrix of X
2. the number of observation
3. the p-values for all pairwise correlations

Correlation matrix

```
library(Hmisc)
X <- as.matrix(X) res <- rcorr(X)
```

```
> str(res)
List of 3
$ r: num [1:11, 1:11] 1 -0.852 -0.848 -0.776 0.681 ...
..- attr(*, "dimnames")=List of 2
.. ..$ : chr [1:11] "mpg" "cyl" "disp" "hp" ...
.. ..$ : chr [1:11] "mpg" "cyl" "disp" "hp" ...
$ n: int [1:11, 1:11] 32 32 32 32 32 32 32 32 32 32 ...
..- attr(*, "dimnames")=List of 2
.. ..$ : chr [1:11] "mpg" "cyl" "disp" "hp" ...
.. ..$ : chr [1:11] "mpg" "cyl" "disp" "hp" ...
$ P: num [1:11, 1:11] NA 6.11e-10 9.38e-10 1.79e-07 1.78e-05 ...
..- attr(*, "dimnames")=List of 2
.. ..$ : chr [1:11] "mpg" "cyl" "disp" "hp" ...
.. ..$ : chr [1:11] "mpg" "cyl" "disp" "hp" ...
- attr(*, "class")= chr "rcorr"
```

Correlation matrix

We are displaying only the matrix of p values, with 3 decimal digits

```
> round(res$P, 3)
```

	mpg	*cyl*	*disp*	*hp*	*drat*	*wt*	*qsec*	*gear*	*carb*
mpg	*NA*	0.000	0.000	0.000	0.000	0.000	0.017	0.005	0.001
cyl	0.000	*NA*	0.000	0.000	0.000	0.000	0.000	0.004	0.002
disp	0.000	0.000	*NA*	0.000	0.000	0.000	0.013	0.001	0.025
hp	0.000	0.000	0.000	*NA*	0.010	0.000	0.000	0.493	0.000
drat	0.000	0.000	0.000	0.010	*NA*	0.000	0.620	0.000	0.621
wt	0.000	0.000	0.000	0.000	0.000	*NA*	0.339	0.000	0.015
qsec	0.017	0.000	0.013	0.000	0.620	0.339	*NA*	0.243	0.000
gear	0.005	0.004	0.001	0.493	0.000	0.000	0.243	*NA*	0.129
carb	0.001	0.002	0.025	0.000	0.621	0.015	0.000	0.129	*NA*

Principal Components Analysis

Principal Components Analysis

Principal Components Analysis (PCA) is a statistical method designed to reduce data dimensionality.

PCA extracts the most significant information from a set of multiple variables and represents this information as a set of new variables, called **principal components**, obtained as linear combinations of the original ones.

PCA allows one to identify a few principal components that can be visualized graphically with minimal loss of information.

The dominant principal components are the most important for explaining covariation in the data.

Principal Components Analysis

PCA differs from clustering which is also used for data interpretation.

- Clustering assumes that each data point is a member of one, and only one, cluster. Clusters are mutually exclusive.
- PCA assumes that each data point is a linear combination of multiple basic "ingredients" which are not mutually exclusive.

Principal Components Analysis

I will use dataset `decathlon2` from the `factoextra` package to illustrate the ue of PCA.

```
> install.packages("factoextra")
> library("factoextra")
> data(decathlon2)
> head(decathlon2)
```

	X100m	L.jump	Shot.put	H.jump	X400m	X110m.hurdle	Discus	Pole.vault	Javeline	X1500m	Rank	Points	Competition
SEBRLE	11.04	7.58	14.83	2.07	49.81	14.69	43.75	5.02	63.19	291.7	1	8217	Decastar
CLAY	10.76	7.40	14.26	1.86	49.37	14.05	50.72	4.92	60.15	301.5	2	8122	Decastar
BERNARD	11.02	7.23	14.25	1.92	48.93	14.99	40.87	5.32	62.77	280.1	4	8067	Decastar
YURKOV	11.34	7.09	15.19	2.10	50.42	15.31	46.26	4.72	63.44	276.4	5	8036	Decastar
ZSIVOCZKY	11.13	7.30	13.48	2.01	48.62	14.17	45.67	4.42	55.37	268.0	7	8004	Decastar
McMULLEN	10.83	7.31	13.76	2.13	49.91	14.38	44.41	4.42	56.37	285.1	8	7995	Decastar

Principal Components Analysis

The dataset `decathlon2` describes athletes' performance during two sporting events (Desctar and OlympicG).

It contains 27 athletes described by 13 variables (sport disciplines).

For further analysis, I will subset active individuals (rows 1:23) and active variables (columns 1:10) from the `decathlon2` dataset, therefore I will create new dataset decathlon2b to conduct the principal component analysis.

```
decathlon2b <- decathlon2[1:23, 1:10]
```

The `decathlon2b` dataset consists of 23 observations and 10 variables.

```
> dim(decathlon2b)
[1] 23 10
```

Principal Components Analysis

The summary statistics below shows the distribution of observations.

```
> summary(decathlon2b)
     X100m         Long.jump        Shot.put       High.jump         X400m
 Min.   :10.44   Min.   :6.800   Min.   :12.68   Min.   :1.860   Min.   :46.81
 1st Qu.:10.84   1st Qu.:7.165   1st Qu.:14.17   1st Qu.:1.940   1st Qu.:48.95
 Median :10.97   Median :7.310   Median :14.65   Median :2.010   Median :49.40
 Mean   :11.00   Mean   :7.350   Mean   :14.62   Mean   :2.007   Mean   :49.43
 3rd Qu.:11.23   3rd Qu.:7.525   3rd Qu.:15.14   3rd Qu.:2.095   3rd Qu.:50.02
 Max.   :11.64   Max.   :7.960   Max.   :16.36   Max.   :2.150   Max.   :51.16
  X110m.hurdle       Discus        Pole.vault       Javeline         X1500m
 Min.   :13.97   Min.   :37.92   Min.   :4.400   Min.   :52.33   Min.   :262.1
 1st Qu.:14.17   1st Qu.:43.74   1st Qu.:4.610   1st Qu.:55.40   1st Qu.:268.8
 Median :14.37   Median :44.75   Median :4.820   Median :57.44   Median :278.1
 Mean   :14.53   Mean   :45.16   Mean   :4.797   Mean   :59.11   Mean   :277.9
 3rd Qu.:14.94   3rd Qu.:46.93   3rd Qu.:5.000   3rd Qu.:62.98   3rd Qu.:283.6
 Max.   :15.67   Max.   :51.65   Max.   :5.320   Max.   :70.52   Max.   :301.5
```

Principal Components Analysis

The R command to perform a principal components analysis on a data matrix x is the following

```
prcomp(x, retx = TRUE, center = TRUE, scale = FALSE,
tol = NULL, ...)
```

- retx: A logical value indicating whether the rotated variables should be returned. The default is TRUE.
- center: A logical value indicating whether the variables should be shifted to be 0 centered. Alternately, a vector of length equal the number of columns of x can be supplied. The value is passed to scale. The default is TRUE.
- scale: A logical value indicating whether the variables should be scaled to have unit variance before the analysis takes place. The default is FALSE. In general, scaling is advisable.
- tol: a value indicating the magnitude below which components should be omitted. With the default NULL setting, no components are omitted.

Principal Components Analysis

```
> res.pca <- prcomp(decathlon2b, scale = TRUE)
> print(res.pca)
```

```
Standard deviations (1, .., p=10):

 [1] 2.0308159 1.3559244 1.1131668 0.9052294 0.8375875 0.6502944 0.5500742
 [8] 0.5238988 0.3939758 0.3492435

Rotation (n x k) = (10 x 10):

                     PC1         PC2         PC3         PC4        PC5
X100m       -0.418859080  0.13230683 -0.27089959  0.03708806 -0.2321476
Long.jump    0.391064807 -0.20713320  0.17117519 -0.12746997  0.2783669
Shot.put     0.361388111 -0.06298590 -0.46497777  0.14191803 -0.2970589
High.jump    0.300413236  0.34309742 -0.29652805  0.15968342  0.4807859
X400m       -0.345478567 -0.21400770 -0.25470839  0.47592968  0.1240569
X110m.hurdle -0.376265119  0.01824645 -0.40325254 -0.01866477  0.2676975
Discus       0.365965721 -0.03662510 -0.15857927  0.43636361 -0.4873988
Pole.vault  -0.106985591 -0.59549862 -0.08449563 -0.37447391 -0.2646712
Javeline     0.210864329 -0.28475723 -0.54270782 -0.36646463  0.2361698
X1500m       0.002106782 -0.57855748  0.19715884  0.49491281  0.3142987
                     PC6         PC7         PC8         PC9        PC10
X100m        0.054398099 -0.16604375 -0.19988005 -0.76924639  0.12718339
Long.jump   -0.051865558 -0.28056361 -0.75850657 -0.13094589  0.08509665
Shot.put    -0.368739186 -0.01797323  0.04649571  0.12129309  0.62263702
High.jump   -0.437716883  0.05118848  0.16111045 -0.28463225 -0.38244596
X400m       -0.075796432  0.52012255 -0.44579641  0.20854176 -0.09784197
X110m.hurdle  0.004048005 -0.67276768 -0.01592804  0.41058421 -0.04475363
Discus       0.305315353 -0.25946615 -0.07550934  0.03391600 -0.49418361
Pole.vault  -0.503563524 -0.01889413  0.06282691 -0.06540692 -0.39288155
Javeline     0.556821016  0.24281145  0.10086127 -0.10268134 -0.01103627
X1500m       0.064663250 -0.20245828  0.37119711 -0.25950868  0.17991689
```

Principal Components Analysis

- The `prcomp()` function was set to center data around 0 by shifting the variables (center = TRUE) and to rescale the variance to 1 (scale = FALSE); data standarization is needed since variables were measured in different scales.
- The `prcomp()` function computed the 10 principal components which also correspond to the number of variables (10 sport disciplines) in the data.
  Recall that data matrix contains 23 observations (athletes) of 10 variables (sport disciplines).
- Each principal component (PC) explains a percentage of the total variance in the data set.

Principal Components Analysis

Each PC explains a percentage of the total variance in the data set.

```
> summary(res.pca)
  Importance of components:
                            PC1    PC2    PC3     PC4     PC5
  Standard deviation     2.0308 1.3559 1.1132 0.90523 0.83759
  Proportion of Variance 0.4124 0.1839 0.1239 0.08194 0.07016
  Cumulative Proportion  0.4124 0.5963 0.7202 0.80213 0.87229
                             PC6     PC7     PC8     PC9   PC10
  Standard deviation     0.65029 0.55007 0.52390 0.39398 0.3492
  Proportion of Variance 0.04229 0.03026 0.02745 0.01552 0.0122
  Cumulative Proportion  0.91458 0.94483 0.97228 0.98780 1.0000
```

- PC1 explains 41.24% of total variance, PC2 explains 18.39% of total variance and so on.
- The Cumulative Proportion section shows that the first 3 PCs explains about 72% of the total variance and the first 4 PCs explains about 80% of the total variance.

Principal Components Analysis

The amount of variation held by each principal component is associated with the **eigenvalues** of the PCA.

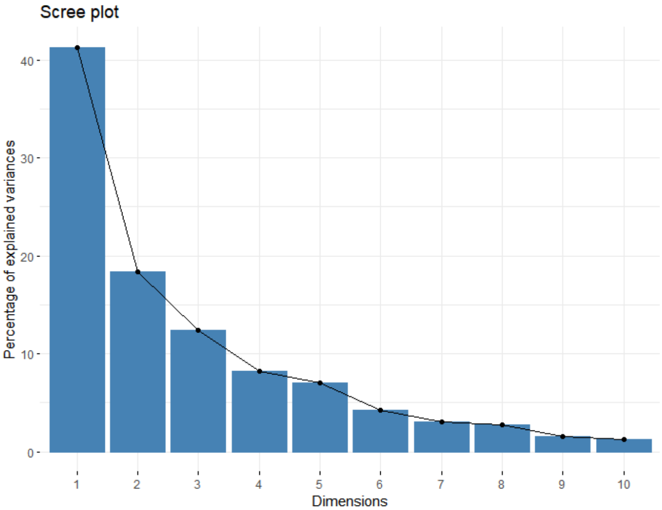
The eigenvalues are extracted by `get_eigenvalue()` function.

```
> eig.val<-get_eigenvalue(res.pca)
> eig.val
        eigenvalue variance.percent cumulative.variance.percent
Dim.1    4.1242133        41.242133                    41.24213
Dim.2    1.8385309        18.385309                    59.62744
Dim.3    1.2391403        12.391403                    72.01885
Dim.4    0.8194402         8.194402                    80.21325
Dim.5    0.7015528         7.015528                    87.22878
Dim.6    0.4228828         4.228828                    91.45760
Dim.7    0.3025817         3.025817                    94.48342
Dim.8    0.2744700         2.744700                    97.22812
Dim.9    0.1552169         1.552169                    98.78029
Dim.10   0.1219710         1.219710                   100.00000
```

Principal Components Analysis

The importance of PCs decreases rapidly with the dimension.

```
> fviz_eig(res.pca, col.var="blue")
```



Principal Components Analysis

The **Scree plot** displays the variance by each PC.

It always displays a downward curve. It typically starts high, then falls rather quickly and finally flattens out. This is because the first component usually explains much of the variability, the next few components explain a moderate amount, and the latter components only explain a small fraction of the overall variability.

The scree plot is useful to decide the number of PCs that are sufficient to provide a satisfactory approximation to explain the data. scree plot criterion looks for the **"elbow"** in the curve and selects all components just before the line flattens out.

Note: it is called a 'scree' plot (in the PCA literature) because it often looks like a 'scree' slope, where rocks have fallen down and accumulated on the side of a mountain.

Principal Components Analysis

PCA results can be assessed with regard to **variables** (sport disciplines) and **observations/individuals** (athletes).

For that purpose, the function `get_pca_var()` provides a list of matrices containing all the results for the **variables**: coordinates, correlation between variables and axes, squared cosine, and contributions.

Similarly, the function `get_pca_ind()` provides a list of matrices containing all the results for the **observations/individuals**: coordinates, squared cosine, and contributions.

Principal Components Analysis

```
> var <- get_pca_var(res.pca)
> var
```

Principal Component Analysis Results for variables

```
===================================
```

	Name	Description
1	"$coord"	"Coordinates for the variables"
2	"$cor"	"Correlations between variables and dimensions"
3	"$cos2"	"Cos2 for the variables"
4	"$contrib"	"contributions of the variables"

```
> ind <- get_pca_ind(res.pca)
> ind
```

Principal Component Analysis Results for individuals

```
===================================
```

	Name	Description
1	"$coord"	"Coordinates for the individuals"
2	"$cos2"	"Cos2 for the individuals"
3	"$contrib"	"contributions of the individuals"

Principal Components Analysis

We start by assessing PCA results with regard to variables.

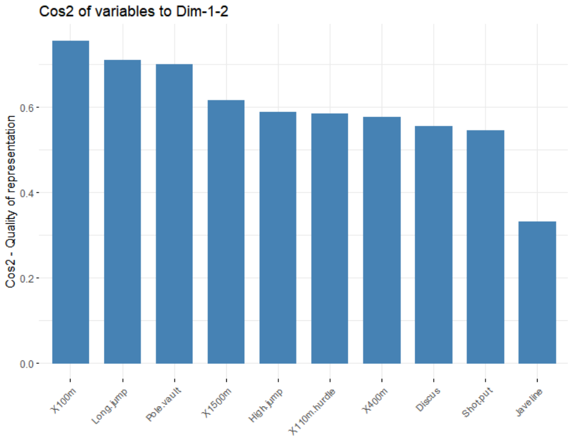
In the list above:

- `Cos2` is called **square cosine** and shows the importance of a principal component for a given observation.
    - A low value means that the variable is not well represented by that component
    - A high value, on the other hand, means a good representation of the variable on that component.
- `Contrib` indicates the **contribution** of the variables.

Principal Components Analysis

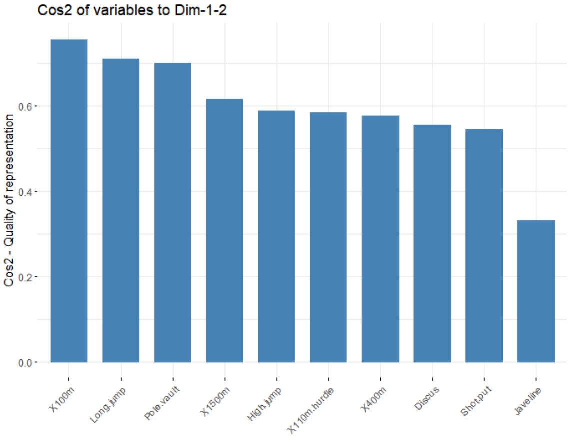
The code below computes the square cosine value for each variable with respect to the first two principal components PC1, PC2.

```
> fviz_cos2(res.pca, choice = "var", axes = 1:2)
```



Principal Components Analysis

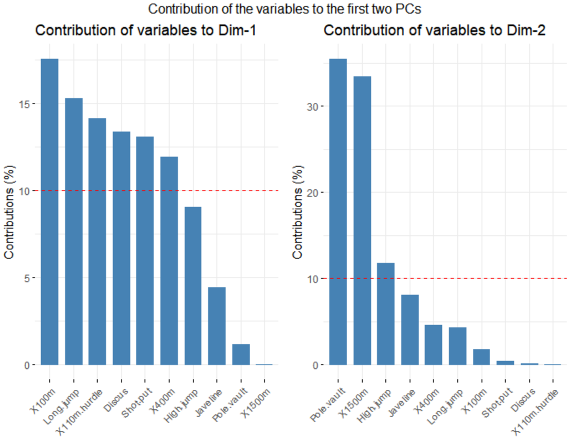
From the plot, X100m, Long jump and Pole vault are the top three variables with the highest cos2, hence they are well represented in PC1 and PC2.



Principal Components Analysis

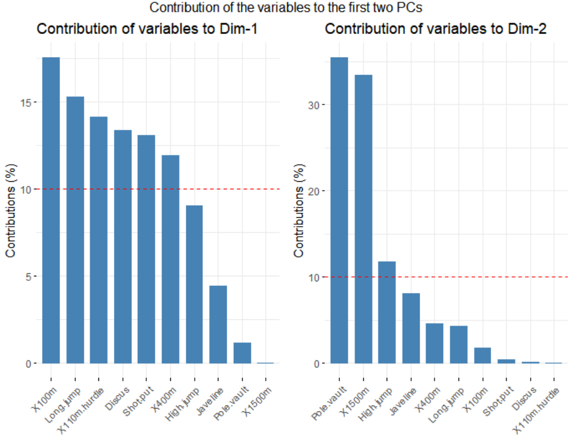
The code below shows variable contributions to PC1 and PC2.

```
> a1<-fviz_contrib(res.pca, choice = "var", axes = 1)

> a2<-fviz_contrib(res.pca, choice = "var", axes = 2)

> library("gridExtra")

> grid.arrange(a1,a2,ncol=2, top='Contribution of the variables to the first two PCs')
```



Principal Components Analysis

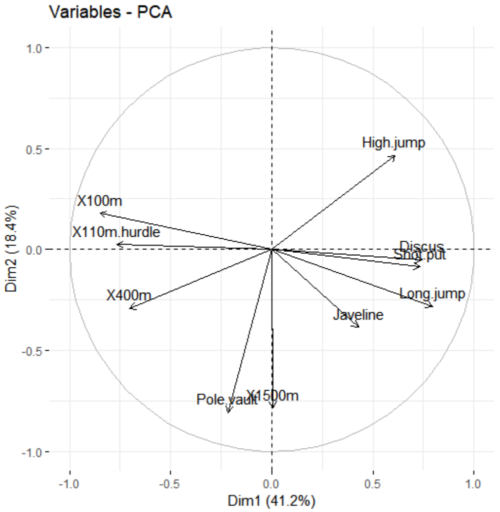
The red dashed line on the graph above indicates the expected average contribution. A variable with a contribution exceeding this benchmark is considered as important in contributing to the PC. It can be seen that the variables X100m, Long.jump and Pole.vault contribute the most to both dimensions.



Principal Components Analysis

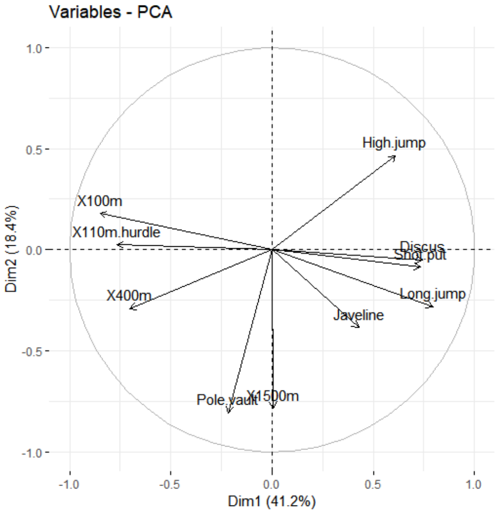
The **biplot** visualizes similarities/dissimilarities between variables.

```
> fviz_pca_var(res.pca, col.var = "black")
```



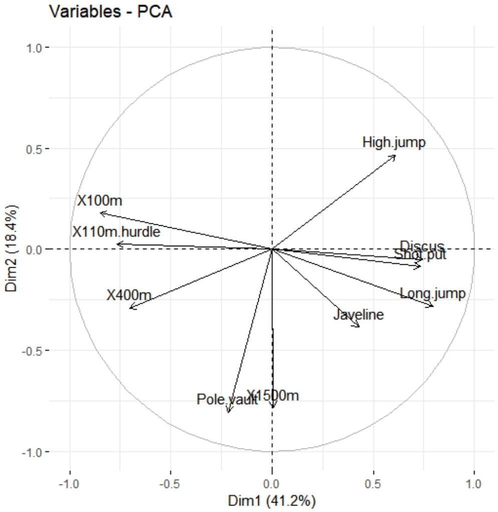
Principal Components Analysis

- Variables that are grouped together are positively correlated to each other and variables that are negatively correlated are displayed to the opposite sides of the biplot's origin.



Principal Components Analysis

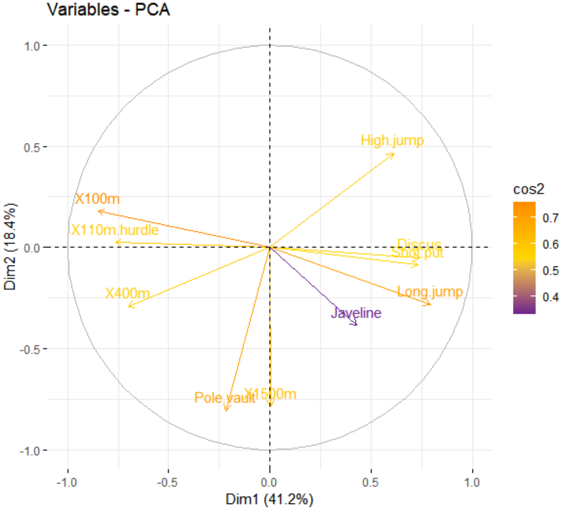
- The higher the distance between the variable and the origin, the better represented that variable is in the principal components PC1 and PC2.



Principal Components Analysis

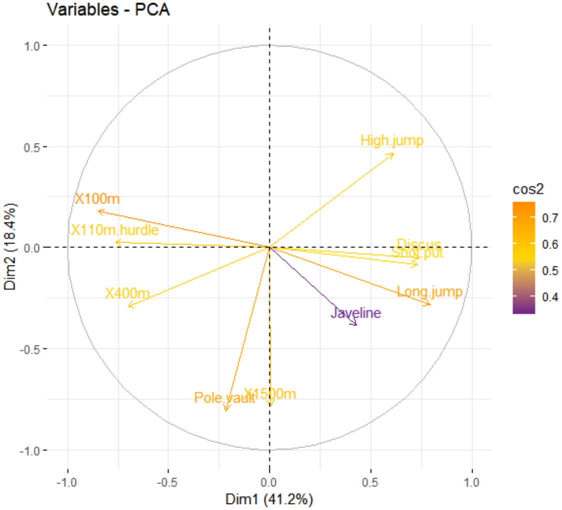
The quality of representation of variables can be drawn on the plot.

```
> fviz_pca_var(res.pca, col.var = "cos2", gradient.cols =
c("darkorchid4", "gold", "darkorange"), )
```



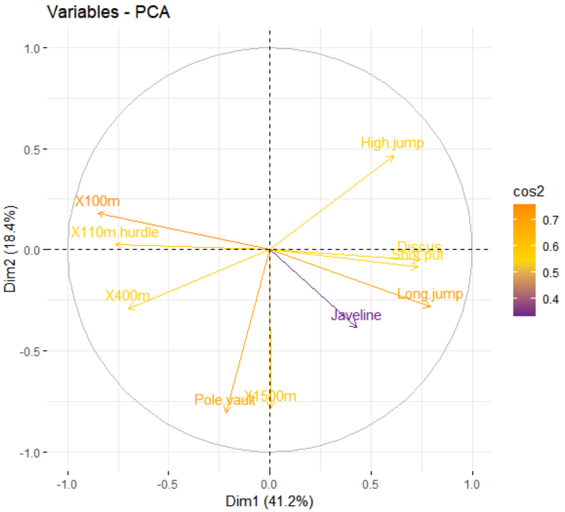
Principal Components Analysis

In the plot, cos2 values differ by gradient colors: variables with low cos2 values are colored “darkorchid4”, medium cos2 values - “gold”, high co2 values - “darkorange”.



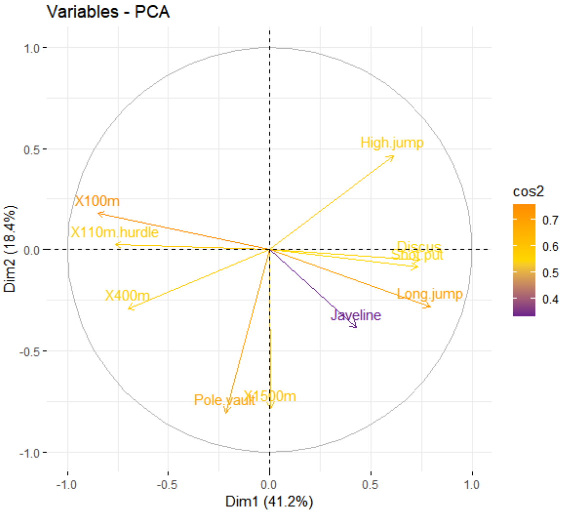
Principal Components Analysis

X100m, Long.jump and Pole.vault have high cos2 implying a good representation on the principal component. Variables are positioned close to the circumference of the correlation circle.



Principal Components Analysis

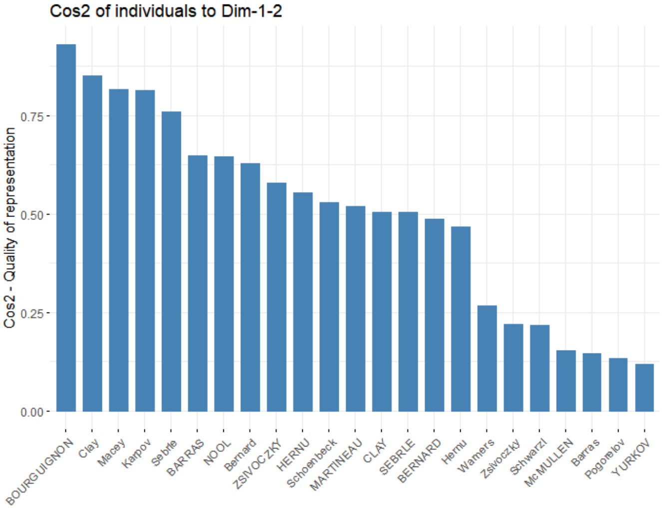
Javeline has the lowest cos2 indicating that the variable is not well represented by the PCs. The variable is close to the center of the circle, so it is less important for the first components.



Principal Components Analysis

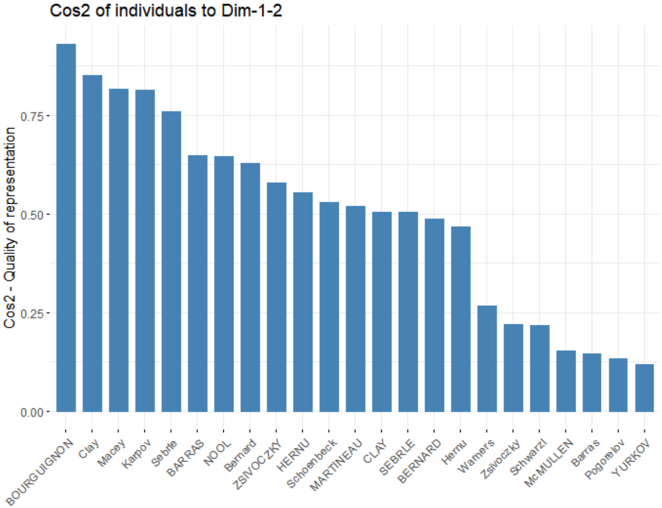
We now similarly assess PCA results with regard to individuals using cos2.

```
> fviz_cos2(res.pca, choice = "ind", axes = 1:2)
```



Principal Components Analysis

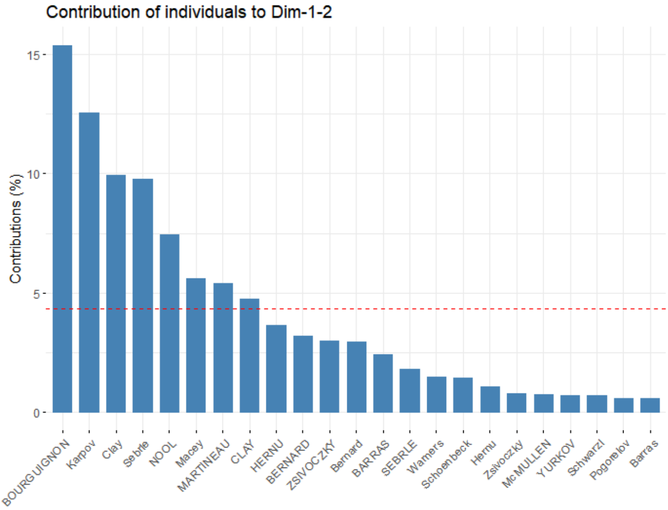
The plot shows the athletes on the left are well represented in PC1, PC2.



Principal Components Analysis

We next assess PCA results for individuals using contrib.

```
> fviz_contrib(res.pca, choice = "ind", axes = 1:2)
```



Principal Components Analysis

The plot shows the athletes contributing the most to PC1, PC2.