# Clustering

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### Introduction

Working in high-dimensional spaces can be undesirable for several reasons so it could be useful to project the features to a space of fewer dimensions.

Principal Component Analysis (PCA) is a *Dimension Reduction* technique for unsupervised problems. It projects/transforms the data into a lower-dimensional space so that the lower-dimensional representation retains some meaningful properties of the original data, ideally close to its intrinsic dimension.

#### Libraries

We are going to use:

- mvtnorm: Multivariate Normal and t Distributions
- factoextra: Extract and Visualize the Results of Multivariate Data Analyses
- scales: Scale Functions for Visualization
- ellipse: Functions for drawing ellipses and ellipse-like confidence regions
- corrplot: Visualization of a Correlation Matrix

```
library(mvtnorm) # for the toy simulated example
library(factoextra) # contains also decathlon data
library(scales) # to create ggplot-like figures in base R (color transparency)
library(ellipse) # to add elliptical confidence regions in base R plots
library(corrplot) # correlation plots
```

#### Data

Today we are going to use the **decathlon2** data set, which is available in the **factoextra** package. It consists of 27 observations (athletes) and the following 13 variables (performance).

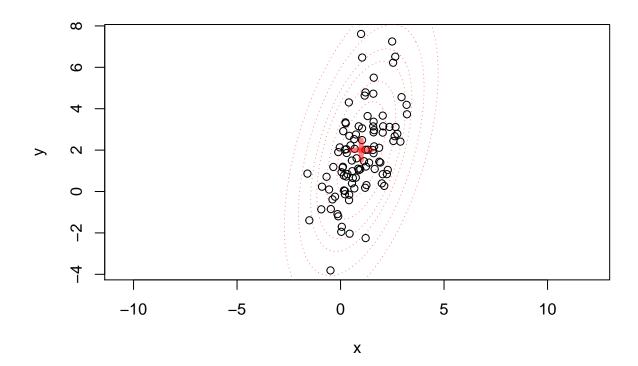
```
help(decathlon2)
head(decathlon2)
             X100m Long.jump Shot.put High.jump X400m X110m.hurdle Discus
## SEBRLE
             11.04
                        7.58
                                14.83
                                           2.07 49.81
                                                              14.69
                                                                     43.75
                        7.40
## CLAY
             10.76
                                14.26
                                           1.86 49.37
                                                              14.05
                                                                     50.72
## BERNARD
             11.02
                        7.23
                                14.25
                                                              14.99 40.87
                                           1.92 48.93
## YURKOV
             11.34
                        7.09
                                15.19
                                           2.10 50.42
                                                              15.31 46.26
## ZSIVOCZKY 11.13
                        7.30
                                13.48
                                           2.01 48.62
                                                              14.17 45.67
## McMULLEN 10.83
                        7.31
                                13.76
                                           2.13 49.91
                                                              14.38 44.41
             Pole.vault Javeline X1500m Rank Points Competition
## SEBRLE
                   5.02
                           63.19 291.7
                                               8217
                                                        Decastar
                                           1
## CLAY
                   4.92
                           60.15 301.5
                                               8122
                                                        Decastar
## BERNARD
                   5.32
                           62.77 280.1
                                           4
                                               8067
                                                        Decastar
## YURKOV
                   4.72
                           63.44 276.4
                                           5
                                               8036
                                                        Decastar
## ZSIVOCZKY
                   4.42
                           55.37 268.0
                                           7
                                               8004
                                                        Decastar
## McMULLEN
                   4.42
                           56.37 285.1
                                               7995
                                                        Decastar
```

# A Toy Example of Dimension Reduction

Let's simulate a 2-dimensional data set from a Gaussian distribution with higher dispersion along the y-axis.

```
set.seed(1234)
                               # set seed for reproducibility
mu <-c(1, 2)
                               # location/mean vector (p times 1)
sig \leftarrow cbind(c(1,1), c(1,4)) + covariance matrix (p times p)
  <- 100
                               # number of points
X <- rmvnorm(n, mu, sig)</pre>
                               # data generation
colnames(X) <- c("x","y")</pre>
                               # renaming
head(X)
                               # visualize our data
##
                  х
## [1,] -0.03816118 2.13170559
## [2,]
        1.21209499 -2.24884418
## [3,]
        1.57692190 3.14455298
## [4,]
        0.27238812 0.72545111
## [5,]
        0.16401245 0.05239442
## [6,] 0.20871312 -0.13108549
plot(X, asp=1)
                               # plot our data (with fixed aspect ratio)
points(mu[1], mu[2],
                               # add centroid
       col=alpha("red", 0.5), # marker color and transparency
       pch=3,
                               # marker type
       lwd=5,
                               # marker width
       cex=2)
                               # marker size
# iterate across confidence levels
conflev \leftarrow c(0.5, 0.75, 0.9, 0.95, 0.99, 0.999)
for (confi in conflev){
  lines(ellipse(sig, centre=mu, level=confi),
                                                   # add elliptical confidence regions
```

```
col = alpha("red", 0.5),  # add color and transparency
lty = 3)  # dashed lines
}
```

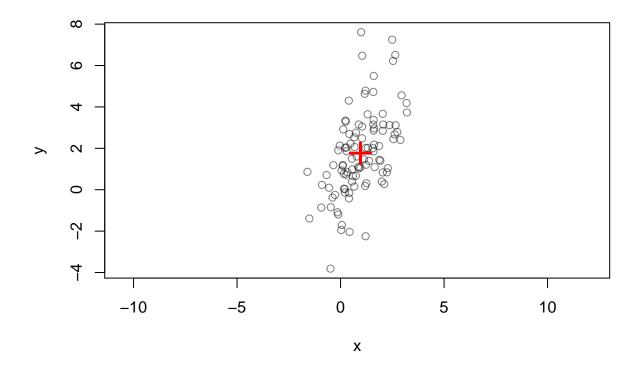


How can we reduce the dimension of these data?

We can reduce the number of features (columns) in different ways. Let's see some.

### Using the sample mean

The sample mean is the easiest 0-dimensional data reduction method, because it allows to collapse all the information into a single point.



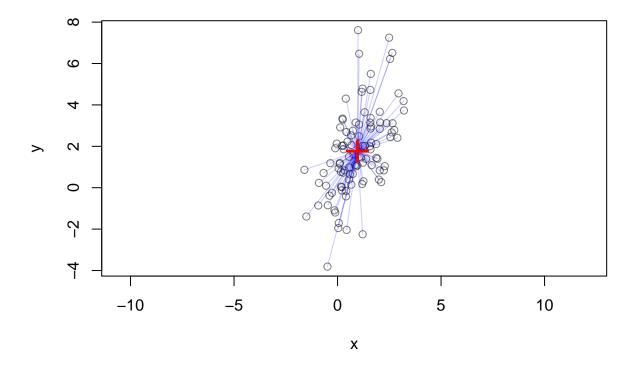
What is the variance?

What is the associated loss of information?

What is the error?

We can think of the error in this way:

```
plot(X, asp=1,
                                # plotting the points
     col=alpha('black', 0.5))
                                # reduce the transparency
for(i in 1:n){
                                # for each point
  lines(rbind(X[i,], med),
                                # plot the "error"
        col=alpha('blue',0.2))
}
points(med[1], med[2],
                                # plotting their centroid
       col='red', pch=3,
                                # color, marker type
       cex = 2, lwd=3)
                                # size, width
```



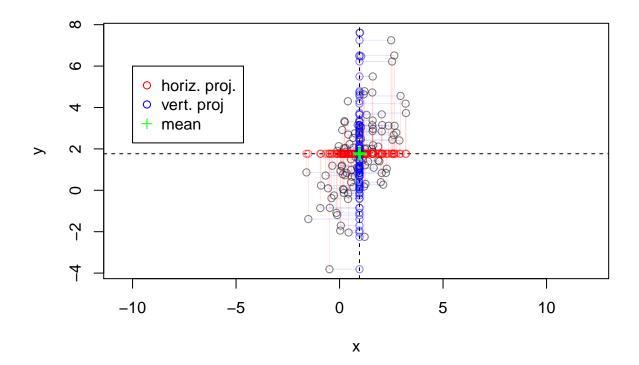
We are collapsing our data to one point, the sample mean (also known as PC0). The error is high.

### Projecting the data on a new axis

We can easily identify two axes from the sample mean: an horizontal-axis, and a vertical-axis.

```
plot(X, asp=1, col=alpha('black', 0.5))
                                             # data
abline(h=med[2], lty=2)
                                             # horizontal axis
points(X[,1], rep(med[2], n),
                                             # projected points
       col=alpha('red',0.5))
abline(v=med[1], lty=2)
                                             # vertical axis
points(rep(med[1], n), X[,2],
                                             # projected points
       col=alpha('blue',0.5))
for(i in 1:n){
  lines(rbind(X[i,], c(X[i,1],med[2])),
                                             # plot the horiz. proj. "error"
        col=alpha('red',0.1))
  lines(rbind(X[i,], c(med[1], X[i,2])),
                                             # plot the vert. proj. "error"
    col=alpha('blue',0.1))
points(med[1], med[2], col='green',
                                             # centroid
       pch=3, cex = 1, lwd=3)
```

```
legend(-10,6,  # legend location
    c("horiz. proj.","vert. proj","mean"),
    col=c("red","blue","green"),
    pch=c(1,1,3))
```

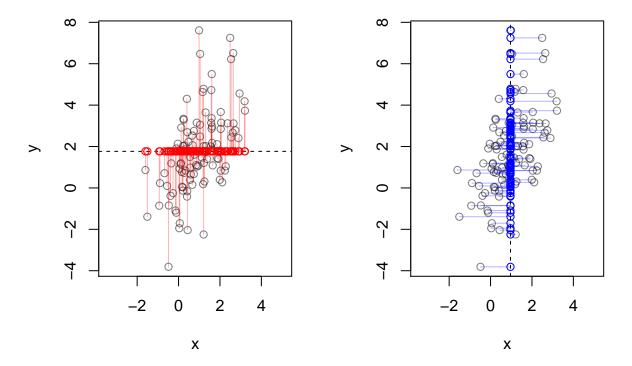


abline(h=med[2], lty=2)

points(X[,1], rep(med[2], n), col='red')

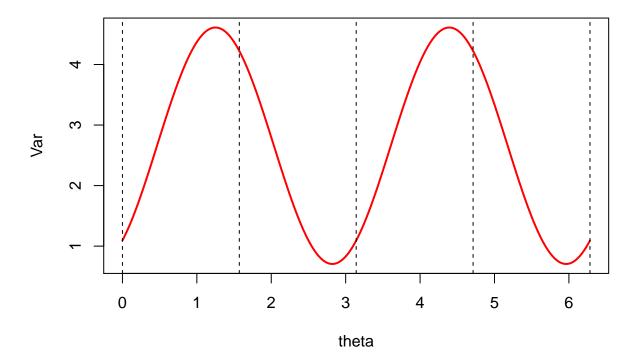
```
for(i in 1:n)
   lines(rbind(X[i,], c(X[i,1], med[2])), col=alpha('red',0.3))

# right panel: vert. axis
plot(X, asp=1, col=alpha('black', 0.5))
abline(v=med[1], lty=2)
points(rep(med[1], n), X[,2], col='blue')
for(i in 1:n)
   lines(rbind(c(med[1],X[i,2]),X[i,]), col=alpha('blue',0.3))
```



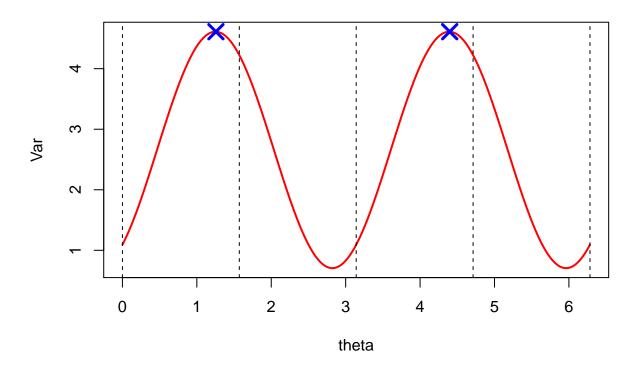
```
# reset it as 1 x 1
par(mfrow=c(1,1))
```

Using this strategy we can find the "best" axis – i.e., the one maximizing the variance. Let's try a brute force approach.



The direction with highest variability is identified by the maximum of the function.

```
max.var <- max(Var) # maximum variance
# max.theta <- theta[which.max(Var)] # theta angle with maximum variance (only the 1st)
max.theta <- theta[Var==max.var] # theta angle with maximum variance (not only the 1st)
max.theta
## [1] 1.256637 4.398230
# projected data (see that their variance is equal to the maximum)
projx <- X %*% c(cos(max.theta[1]), sin(max.theta[1]))
var(projx)
## [1,1]
## [1,1] 4.611209
max.var</pre>
## [1] 4.611209
```

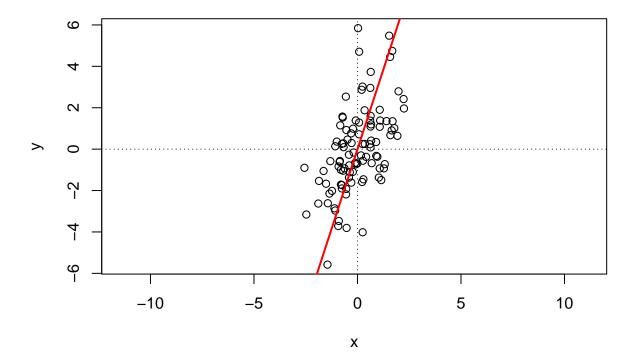


We just found the first principal component (PC1) as the axis maximizing the variance. Let's plot the solution we have found.

Remark: there is rotational invariance, so we can pick any maximizer theta (e.g., the first one).

```
# slope
slopepc1 <- sin(max.theta[1])/cos(max.theta[1])

# plot centered data
plot(Xc, asp=1, col='black')
abline(v=0, lty=3)
abline(h=0, lty=3)
# plot PC1
abline(a=0,b=slopepc1, col = "red", lty=1, lwd=2)</pre>
```

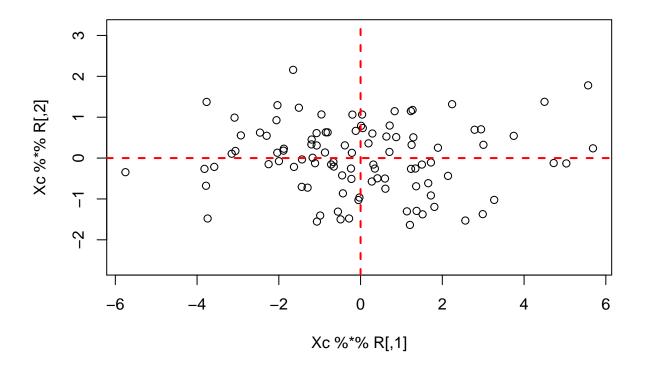


Note that there is only another component orthogonal to PC1 (and centered at 0) since we are in a 2-dimensional setting.

Thus, we can also view PCA as a change of bases/rotation.

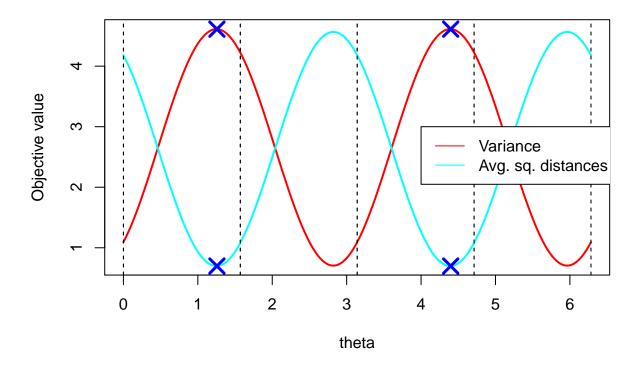
```
# rotation matrix
R1 <- c(cos(max.theta[1]), -sin(max.theta[1]))
R2 <- c(sin(max.theta[1]), cos(max.theta[1]))
R <- rbind(R1, R2)

# plot rotated data such that PC1 and PC2 are now the "standard" bases
plot(Xc %*% R, asp=1)
abline(v=0, col="red",lty=2, lwd=2)
abline(h=0, col="red",lty=2, lwd=2)</pre>
```



Finally, notice that maximizing the variance is equivalent to minimizing squared distances.

```
# Compute the squared distances across (almost) all possible directions
theta2
         \leftarrow seq(0, 2*pi, by = 2*pi/360) # angles
Dist
        <- rep(NA, length(theta))
for(i in 1:length(theta))
                                         # for each angle theta
  mi = sin(theta2[i])/cos(theta2[i])
                                         # slope of the associated line
  distk = rep(NA, n)
                                         # initialize point-to-line distances
  for (k in 1:n){
                                         # compute them
    distk[k] = abs(-mi*Xc[k,1]+Xc[k,2])/sqrt(mi^2+1)
 Dist[i] = mean(distk^2)
                                         # store average of squared distances
# min and argmin for the distance method
           <- min(Dist)
                                                    # min distance
min.dist
min.theta2 <- theta2[Dist==min.dist]</pre>
                                                    # theta angle with min distances
# compare the two approaches
# plotting the Variance for each direction/angle
plot(theta, Var, type = 'l', col='red',
     lwd = 2, lty=1, ylab = "Objective value")
abline(v=c(0, pi/2, pi, 3/2*pi, 2*pi), lty=2)
                                                    # fundamental angles
points(max.theta, rep(max.var, length(max.theta)),
```



Global minima/maxima do differ, but are the arguments (theta values) minimizing/maximizing these functions the same?

```
max.theta
```

```
## [1] 1.256637 4.398230
min.theta2
```

## [1] 1.256637 4.398230

The same result can be obtained through low-rank approximations.

The function **princomp()** in the **stats** package uses the spectral decomposition, **prcomp()** which is part of

the package FactoMineR uses the singular value decomposition (SVD). We will focus on the latter.

### PCA on decathlon2 data

We are going to perform PCA to the first 10 columns of the **decathlon2** data set to analyze athletes performance.

```
# select only the first 10 columns
decathlon2<- decathlon2[, 1:10]
head(decathlon2)
             X100m Long.jump Shot.put High.jump X400m X110m.hurdle Discus
                                             2.07 49.81
## SEBRLE
             11.04
                         7.58
                                 14.83
                                                                14.69
                                                                        43.75
## CLAY
             10.76
                         7.40
                                 14.26
                                             1.86 49.37
                                                                14.05
                                                                        50.72
## BERNARD
             11.02
                         7.23
                                 14.25
                                             1.92 48.93
                                                                14.99
                                                                        40.87
## YURKOV
             11.34
                         7.09
                                 15.19
                                             2.10 50.42
                                                                15.31
                                                                        46.26
## ZSIVOCZKY 11.13
                         7.30
                                 13.48
                                                                        45.67
                                             2.01 48.62
                                                                14.17
## McMULLEN
             10.83
                         7.31
                                 13.76
                                             2.13 49.91
                                                                14.38
                                                                        44.41
##
             Pole.vault Javeline X1500m
## SEBRLE
                    5.02
                            63.19
                                   291.7
                    4.92
## CLAY
                            60.15
                                   301.5
## BERNARD
                    5.32
                            62.77
                                    280.1
## YURKOV
                    4.72
                            63.44
                                   276.4
## ZSIVOCZKY
                    4.42
                            55.37
                                   268.0
## McMULLEN
                            56.37
                                   285.1
                    4.42
dim(decathlon2)
## [1] 27 10
```

```
summary(decathlon2)
```

```
##
        X100m
                       Long.jump
                                          Shot.put
                                                          High.jump
##
    Min.
            :10.44
                             :6.800
                                               :12.68
                                                                :1.860
                     Min.
                                       Min.
                                                        Min.
    1st Qu.:10.84
                     1st Qu.:7.210
                                       1st Qu.:14.17
                                                        1st Qu.:1.930
    Median :10.97
                     Median :7.310
                                       Median :14.57
##
                                                        Median :1.980
                             :7.365
##
    Mean
            :10.99
                     Mean
                                       Mean
                                               :14.54
                                                        Mean
                                                                :1.998
##
    3rd Qu.:11.13
                     3rd Qu.:7.545
                                       3rd Qu.:15.01
                                                        3rd Qu.:2.080
##
    Max.
            :11.64
                     Max.
                             :7.960
                                       Max.
                                               :16.36
                                                        Max.
                                                                :2.150
        X400m
                      X110m.hurdle
##
                                           Discus
                                                          Pole.vault
                                                                :4.400
##
            :46.81
                     Min.
                             :13.97
                                               :37.92
                                                        Min.
    Min.
                                       Min.
##
    1st Qu.:48.70
                     1st Qu.:14.15
                                       1st Qu.:42.27
                                                        1st Qu.:4.660
##
    Median :49.20
                     Median :14.34
                                       Median :44.72
                                                        Median :4.900
##
    Mean
            :49.31
                     Mean
                             :14.50
                                       Mean
                                               :44.85
                                                        Mean
                                                                :4.836
##
    3rd Qu.:49.86
                     3rd Qu.:14.87
                                       3rd Qu.:46.93
                                                        3rd Qu.:5.000
##
    Max.
            :51.16
                     Max.
                             :15.67
                                       Max.
                                               :51.65
                                                        Max.
                                                                :5.400
                          X1500m
##
       Javeline
##
    Min.
            :50.31
                     Min.
                             :262.1
##
    1st Qu.:55.32
                     1st Qu.:271.6
    Median :57.19
                     Median :278.1
##
    Mean
            :58.32
                     Mean
                             :278.5
    3rd Qu.:62.05
                     3rd Qu.:283.6
    Max.
            :70.52
                     Max.
                             :301.5
##
```

To perform PCA we use the function **prcomp**.

```
help(prcomp)
```

##

## \$ x ## ..-

Among other things, the function takes as input:

- data: a data frame
- scale: a logical value (TRUE/FALSE) indicating whether the variables should be scaled to have unit variance before the analysis takes place

Note that by default variables are centered to have zero mean.

Therefore, to perform PCA after scaling the data, we run:

```
res <- prcomp(decathlon2, scale = TRUE)
str(res)
## List of 5
              : num [1:10] 1.936 1.321 1.232 1.016 0.786 ...
   $ rotation: num [1:10, 1:10] -0.423 0.392 0.369 0.314 -0.332 ...
##
    ..- attr(*, "dimnames")=List of 2
    ....$ : chr [1:10] "X100m" "Long.jump" "Shot.put" "High.jump" ...
##
     ....$ : chr [1:10] "PC1" "PC2" "PC3" "PC4" ...
##
   $ center : Named num [1:10] 10.99 7.36 14.54 2 49.31 ...
##
    ..- attr(*, "names")= chr [1:10] "X100m" "Long.jump" "Shot.put" "High.jump" ...
##
##
   $ scale : Named num [1:10] 0.2817 0.2944 0.8364 0.0956 0.9773 ...
```

..- attr(\*, "names")= chr [1:10] "X100m" "Long.jump" "Shot.put" "High.jump" ...

The result is a list containing 5 elements:

• sdev: the standard deviations of the principal components (square root of the eigenvalues)

: num [1:27, 1:10] 0.273 0.888 -1.347 -0.911 -0.102 ...

....\$ : chr [1:27] "SEBRLE" "CLAY" "BERNARD" "YURKOV" ...

• rotation: the matrix of variable loadings (eigenvectors)

....\$ : chr [1:10] "PC1" "PC2" "PC3" "PC4" ...

• center: the centering used if scale=TRUE

..- attr(\*, "dimnames")=List of 2

- attr(\*, "class")= chr "prcomp"

- scale: the scaling used if scale=TRUE
- x: the scores, i.e. the rotated data

# Selecting the number of components

The selection of a "suitable" number of components is non-trivial since in unsupervised learning tasks no ground-truth/labels/response variable is available (which may be used to assess and validate our results otherwise, e.g. through cross-validation – more on this later).

However, some "rules of thumb" have been developed. For instance, one may consider the **percentage of variance explained** (**PVE**), or the **cumulative PVE**.

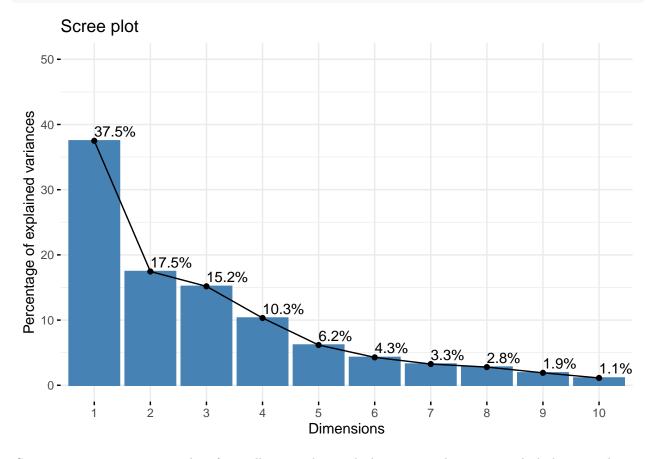
```
help(get_eig)
# eigenvalue, PVE and cumulative PVE for each PC
get_eig(res)

## eigenvalue variance.percent cumulative.variance.percent
## Dim.1 3.7499727 37.499727 37.49973
## Dim.2 1.7451681 17.451681 54.95141
```

```
## Dim.3
           1.5178280
                             15.178280
                                                            70.12969
## Dim.4
           1.0322001
                             10.322001
                                                            80.45169
           0.6178387
## Dim.5
                              6.178387
                                                            86.63008
           0.4282908
                              4.282908
## Dim.6
                                                            90.91298
## Dim.7
           0.3259103
                              3.259103
                                                            94.17209
## Dim.8
           0.2793827
                                                            96.96591
                              2.793827
## Dim.9
           0.1911128
                              1.911128
                                                            98.87704
## Dim.10
           0.1122959
                                                           100.00000
                              1.122959
```

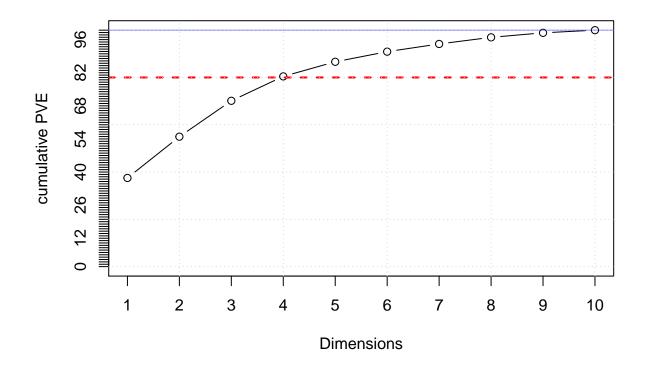
Based on this information we can create a **Scree plot**, and try to find an elbow (i.e. an inflection point) therein.

```
fviz_eig(res, addlabels = TRUE, ylim = c(0, 50))
```



Sometimes, it is not easy to identify an elbow, or this might be associated to a particularly low cumulative PVE.

Thus, it is common fix a priori an acceptance threshold (e.g. 80%) and look at the cumulative PVE.



## Loadings interpretation

Let's focus on the loadings, i.e., the eigenvectors representing the directions of the PCs.

```
loadings <- res$rotation
loadings</pre>
```

```
##
                         PC1
                                    PC2
                                                 PC3
                                                              PC4
                                                                         PC5
                              0.2594748 -0.081870461
## X100m
                -0.42290657
                                                      0.09974877 -0.2796419
## Long.jump
                 0.39189495 -0.2887806
                                         0.005082180 -0.18250903
                                                                   0.3355025
## Shot.put
                 0.36926619
                              0.2135552 -0.384621732
                                                      0.03553644 -0.3544877
## High.jump
                 0.31422571
                              0.4627797 -0.003738604
                                                      0.07012348
                                                                   0.3824125
## X400m
                -0.33248297
                             0.1123521 -0.418635317
                                                      0.26554389
                                                                   0.2534755
## X110m.hurdle -0.36995919
                             0.2252392 -0.338027983 -0.15726889
                                                                   0.2048540
## Discus
                 0.37020078
                             0.1547241 -0.219417086
                                                      0.39137188
                                                                 -0.4319091
## Pole.vault
                -0.11433982 -0.5583051 -0.327177839 -0.24759476
                                                                  -0.3340758
## Javeline
                 0.18341259
                              0.0745854 -0.564474643 -0.47792535
                                                                   0.1697426
## X1500m
                 0.03599937 -0.4300522 -0.286328973
                                                      0.64220377
                                                                   0.3227349
                        PC6
##
                                     PC7
                                                 PC8
                                                              PC9
                                                                         PC10
## X100m
                 0.16023494 -0.03227949
                                          0.35266427 -0.71190625
                                                                   0.03272397
                             0.24902853
                                          0.72986071 -0.12801382
## Long.jump
                 0.07384658
                                                                   0.02395904
## Shot.put
                 0.32207320
                             0.23059438 -0.01767069
                                                      0.07184807
                                                                  -0.61708920
## High.jump
                 0.52738027
                              0.03992994 -0.25003572 -0.14583529
                                                                   0.41523052
## X400m
                              0.69014364 -0.01543618
                                                      0.13706918
                -0.23884715
                                                                   0.12016951
## X110m.hurdle
                 0.26249611 -0.42797378
                                         0.36415520
                                                      0.49550598 -0.03514180
## Discus
                -0.28217086 -0.18416631 0.26865454
                                                      0.18621144
                                                                   0.48037792
```

```
## Pole.vault 0.43606610 0.12654370 -0.16086549 0.02983660 0.40290423 ## Javeline -0.42368592 -0.23324548 -0.19922452 -0.33300936 0.02100398 ## X1500m 0.10850981 -0.34406521 -0.09752169 -0.19899138 -0.18954698
```

We can plot the first two PCs (PC1 and PC2) in the graph of variables (also called correlation circle).

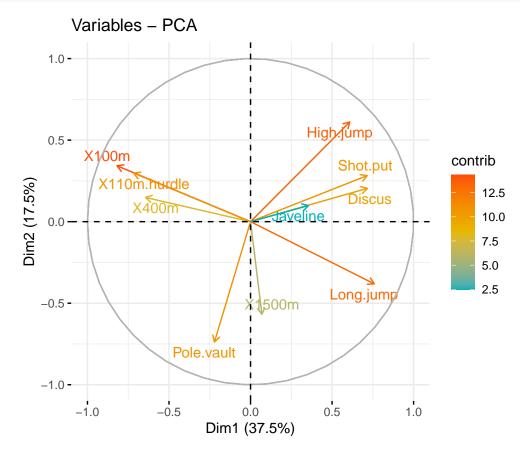
Here the importance of the original features is represented by the **color code**:

red: highblue: mediumwhite: low

and by the length of the vector (its *closeness* to the circle).

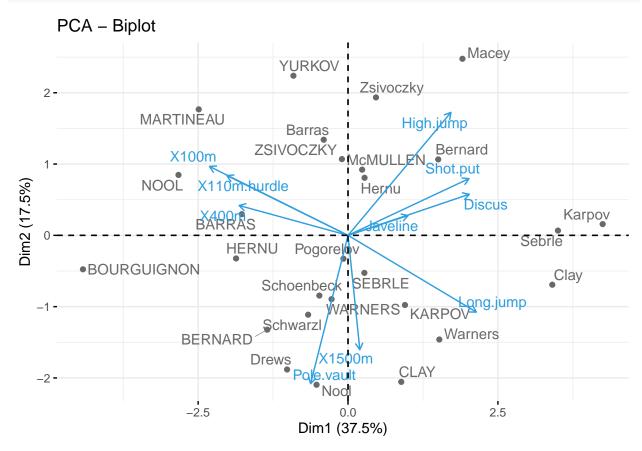
In these plots, positively correlated variables have same direction (they are close to each other, i.e. they have a small angle in between). Negatively correlated variables have opposite directions. Uncorrelated variables are orthogonal.

*Remark:* a lower value for "X100m", "X400m", "X110m hurdle" means a better performance. So it makes sense that they are negatively correlated with "long jump".



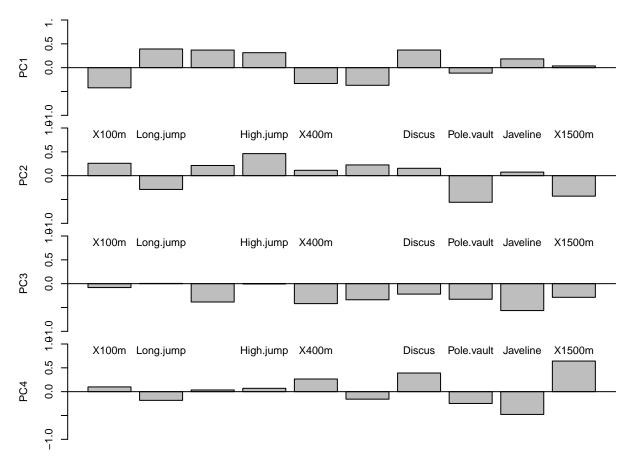
We also see that "X100m", "Long jump" and "High jump" and "Pole vault" contribute the most to PC1 and PC2.

If we want to show also the individuals we can run the **biplot of individuals and variables**. Here similar athletes are grouped together.



Along PC1 we tend to find athletes with higher/lower overall performance, which are mainly related to agility. On PC2 we can distinguish stronger athletes from others.

Remark: observations are represented by their projections, but variables are represented by their correlations. Information regarding all the PCs (e.g., the first 4) can be obtained in the following way:

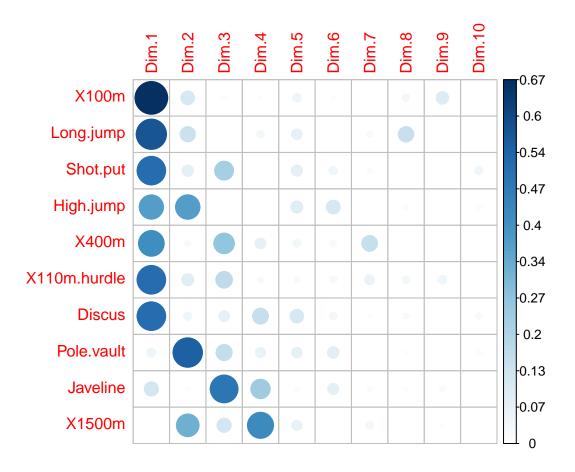


The "importance" of each variable across different PCs is also contained in the field **cos2** of the function get\_pca\_var:

- A high cos2 indicates a good representation of the variable on the principal component. In this case the variable is positioned close to the circumference of the correlation circle.
- A low cos2 indicates that the variable is not perfectly represented by the PCs. In this case the variable is close to the center of the circle.

For a given variable, the sum of the cos2 on all the principal components is equal to one.

```
help(get_pca_var)
varpca <- get_pca_var(res)</pre>
varpca
## 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"
corrplot(varpca$cos2, is.corr=FALSE)
```



# **Multidimensional Scaling**

Multidimensional scaling (MDS) is useful to visualize the level of similarity of individual cases in a dataset. MDS is used to translate "information about the pairwise 'distances' among a set of "n" objects or individuals" into a configuration of "n" points mapped into an abstract Cartesian space.

#### See for instance:

- cmdscale() [stats package]: Classical (metric) multidimensional scaling.
- isoMDS() [MASS package]: Kruskal's non-metric multidimensional scaling (one form of non-metric MDS).
- sammon() [MASS package]: Sammon's non-linear mapping (one form of non-metric MDS).

These functions require a distance object as input and the number of dimensions in the reduced space (by default equal to 2).