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Articles - Principal Component Methods in R: Practical Guide

Principal Component Analysis in R: prcomp vs princomp

 [kassambara](#) |  08/10/2017 |  373276 |  [Comments \(4\)](#) |  [Principal Component Methods in R: Practical Guide](#)

This R tutorial describes how to perform a **Principal Component Analysis (PCA)** using the built-in R functions **prcomp()** and **princomp()**. You will learn how to *predict* new individuals and variables coordinates using PCA. We'll also provide the theory behind *PCA results*.

Learn more about the basics and the interpretation of principal component analysis in our previous article: [PCA - Principal Component Analysis Essentials](#).

PCA in R

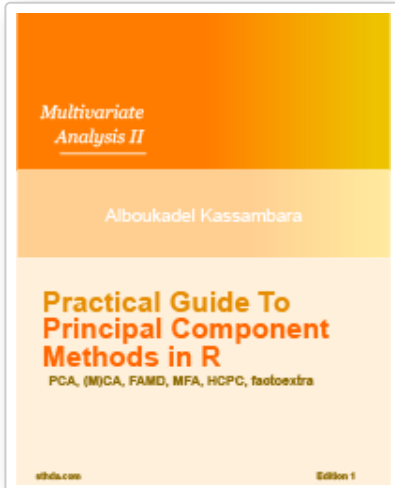
prcomp() vs princomp()

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Related Book:



[Practical Guide to Principal Component Methods in R](#)

General methods for principal component analysis

There are two general methods to perform PCA in R :

- *Spectral decomposition* which examines the covariances / correlations between variables
- *Singular value decomposition* which examines the covariances / correlations between individuals

The function **princomp()** uses the spectral decomposition approach. The functions **prcomp()** and **PCA()** [FactoMineR] use the singular value decomposition (SVD).



According to the R help, SVD has slightly better numerical accuracy. Therefore, the function `prcomp()` is preferred compared to `princomp()`.

prcomp() and princomp() functions

The simplified format of these 2 functions are :

```
prcomp(x, scale = FALSE)
princomp(x, cor = FALSE, scores = TRUE)
```

1. Arguments for **prcomp()**:

- **x**: a numeric matrix or data frame

- **scale**: a logical value indicating whether the variables should be scaled to have unit variance before the analysis takes place

2. Arguments for **princomp()**:

- **x**: a numeric matrix or data frame
- **cor**: a logical value. If TRUE, the data will be centered and scaled before the analysis
- **scores**: a logical value. If TRUE, the coordinates on each principal component are calculated

The elements of the outputs returned by the functions `prcomp()` and `princomp()` includes :

prcomp() name	princomp() name	Description
sdev	sdev	the standard deviations of the principal components
rotation	loadings	the matrix of variable loadings (columns are eigenvectors)
center	center	the variable means (means that were subtracted)
scale	scale	the variable standard deviations (the scaling applied to each variable)
x	scores	The coordinates of the individuals (observations) on the principal components.



In the following sections, we'll focus only on the function **prcomp()**

Package for PCA visualization

We'll use the [factoextra](#) R package to create a ggplot2-based elegant visualization.

- You can install it from CRAN:

```
install.packages("factoextra")
```

- Or, install the latest developmental version from github:

```
if(!require(devtools)) install.packages("devtools")
devtools::install_github("kassambara/factoextra")
```

- Load factoextra as follow:

```
library(factoextra)
```

Demo data sets

We'll use the data sets **decathlon2** [in factoextra], which has been already described at: [PCA - Data format](#).

Briefly, it contains:

- Active individuals (rows 1 to 23) and active variables (columns 1 to 10), which are used to perform the principal component analysis

- Supplementary individuals (rows 24 to 27) and supplementary variables (columns 11 to 13), which coordinates will be predicted using the PCA information and parameters obtained with active individuals/variables.

name	100m	Long.jump	//	Javeline	1500m	Rank	Points	Competition
SEBRLE	11.04	7.58		63.19	291.7	1	8217	Decastar
CLAY	10.76	7.4		60.15	301.5	2	8122	Decastar
Macey	10.89	7.47		58.46	265.42	4	8414	OlympicG
Warners	10.62	7.74		55.39	278.05	5	8343	OlympicG
\\								
Zsivoczky	10.91	7.14		63.45	269.54	6	8287	OlympicG
Hernu	10.97	7.19		57.76	264.35	7	8237	OlympicG
Pogorelov	10.95	7.31		53.45	287.63	11	8084	OlympicG
Schoenbeck	10.9	7.3		60.89	278.82	12	8077	OlympicG
Barras	11.14	6.99		64.55	267.09	13	8067	OlympicG
KARPOV	11.02	7.3		50.31	300.2	3	8099	Decastar
WARNERS	11.11	7.6		51.77	278.1	6	8030	Decastar
Nool	10.8	7.53		61.33	276.33	8	8235	OlympicG
Drews	10.87	7.38		51.53	274.21	19	7926	OlympicG

	Active individuals
	Active variables
	Supplementary quantitative variables
	Supplementary qualitative variable
	Supplementary individuals

Load the data and extract only active individuals and variables:

```
library("factoextra")
data(decathlon2)
decathlon2.active <- decathlon2[1:23, 1:10]
head(decathlon2.active[, 1:6])
```

```
##           X100m Long.jump Shot.put High.jump X400m X110m.hurdle
## SEBRLE      11.0      7.58    14.8      2.07    49.8      14.7
## CLAY        10.8      7.40    14.3      1.86    49.4      14.1
## BERNARD     11.0      7.23    14.2      1.92    48.9      15.0
## YURKOV      11.3      7.09    15.2      2.10    50.4      15.3
## ZSIVOCZKY   11.1      7.30    13.5      2.01    48.6      14.2
## McMULLEN    10.8      7.31    13.8      2.13    49.9      14.4
```

Compute PCA in R using prcomp()

In this section we'll provide an easy-to-use R code to compute and visualize PCA in R using the prcomp() function and the factoextra package.

1. Load factoextra for visualization

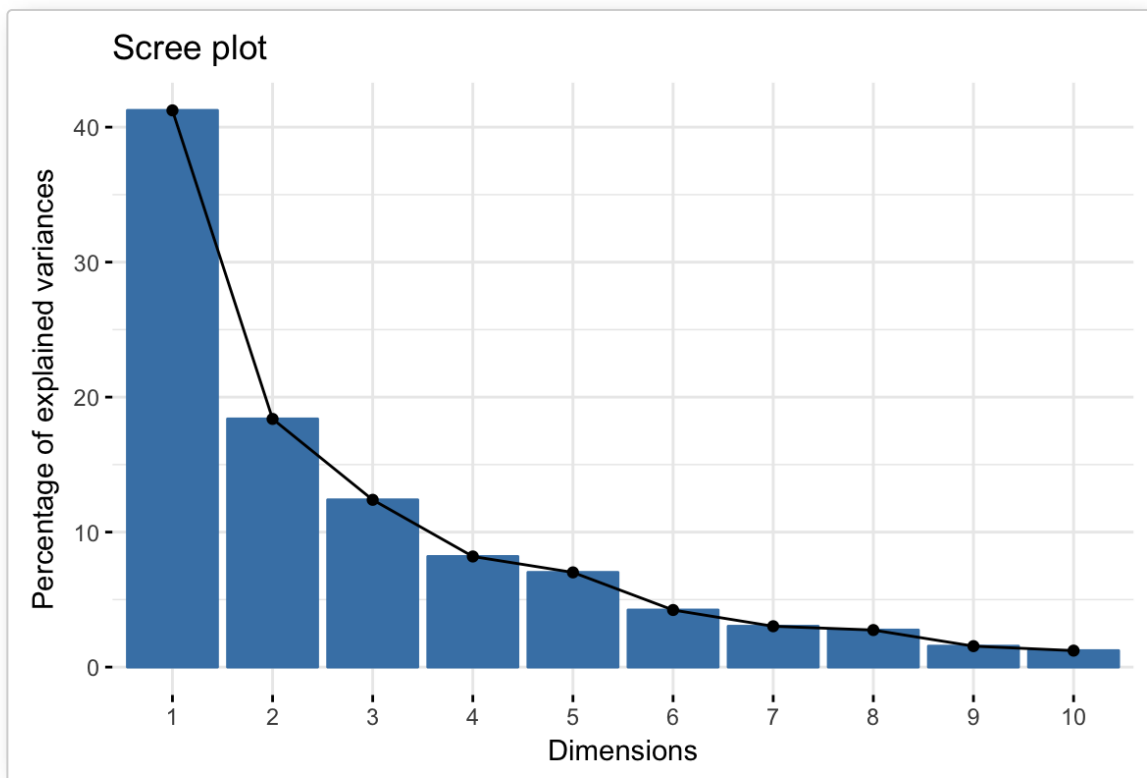
```
library(factoextra)
```

2. Compute PCA

```
res.pca <- prcomp(decathlon2.active, scale = TRUE)
```

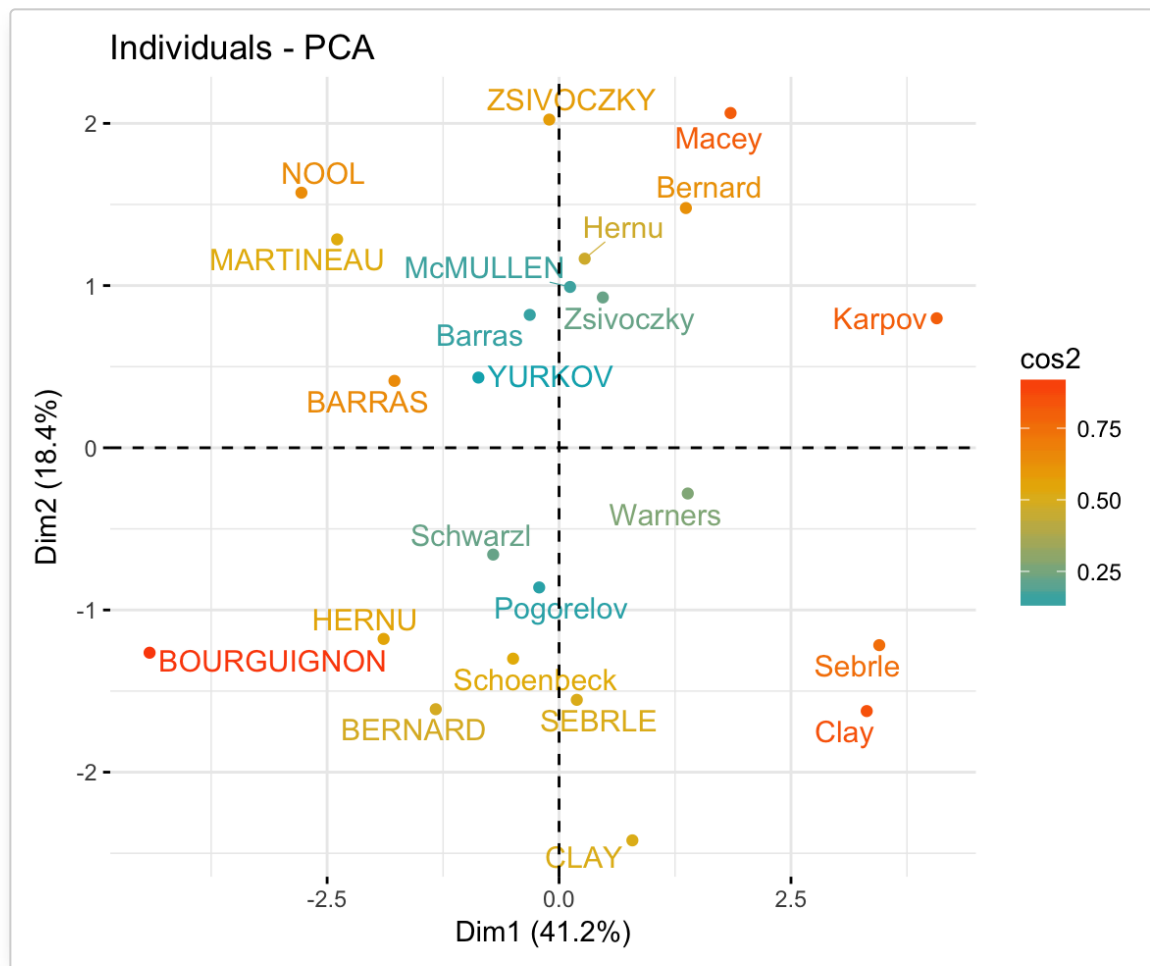
3. Visualize *eigenvalues* (scree plot). Show the percentage of variances explained by each principal component.

```
fviz_eig(res.pca)
```



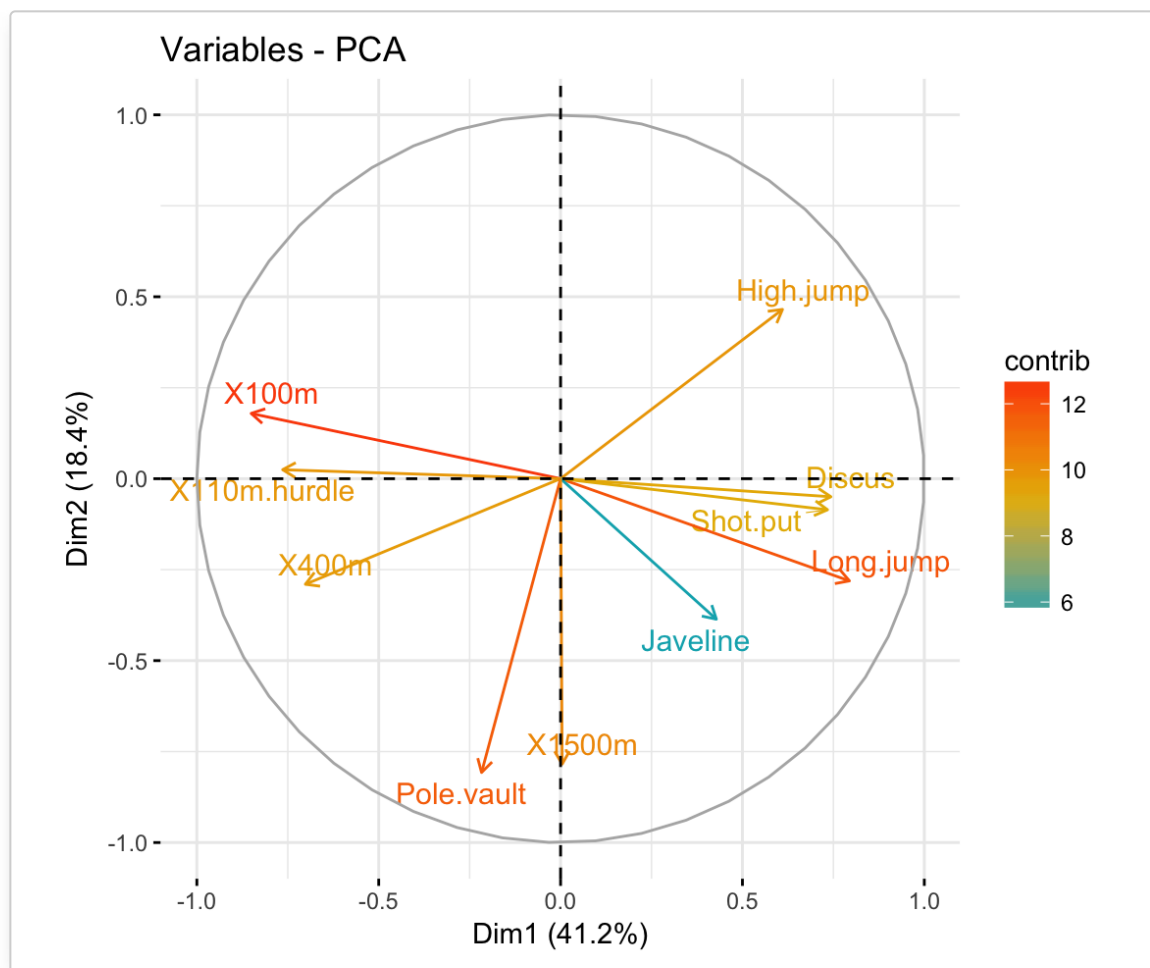
4. Graph of individuals. Individuals with a similar profile are grouped together.

```
fviz_pca_ind(res.pca,  
  col.ind = "cos2", # Color by the quality of representation  
  gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"),  
  repel = TRUE      # Avoid text overlapping  
)
```



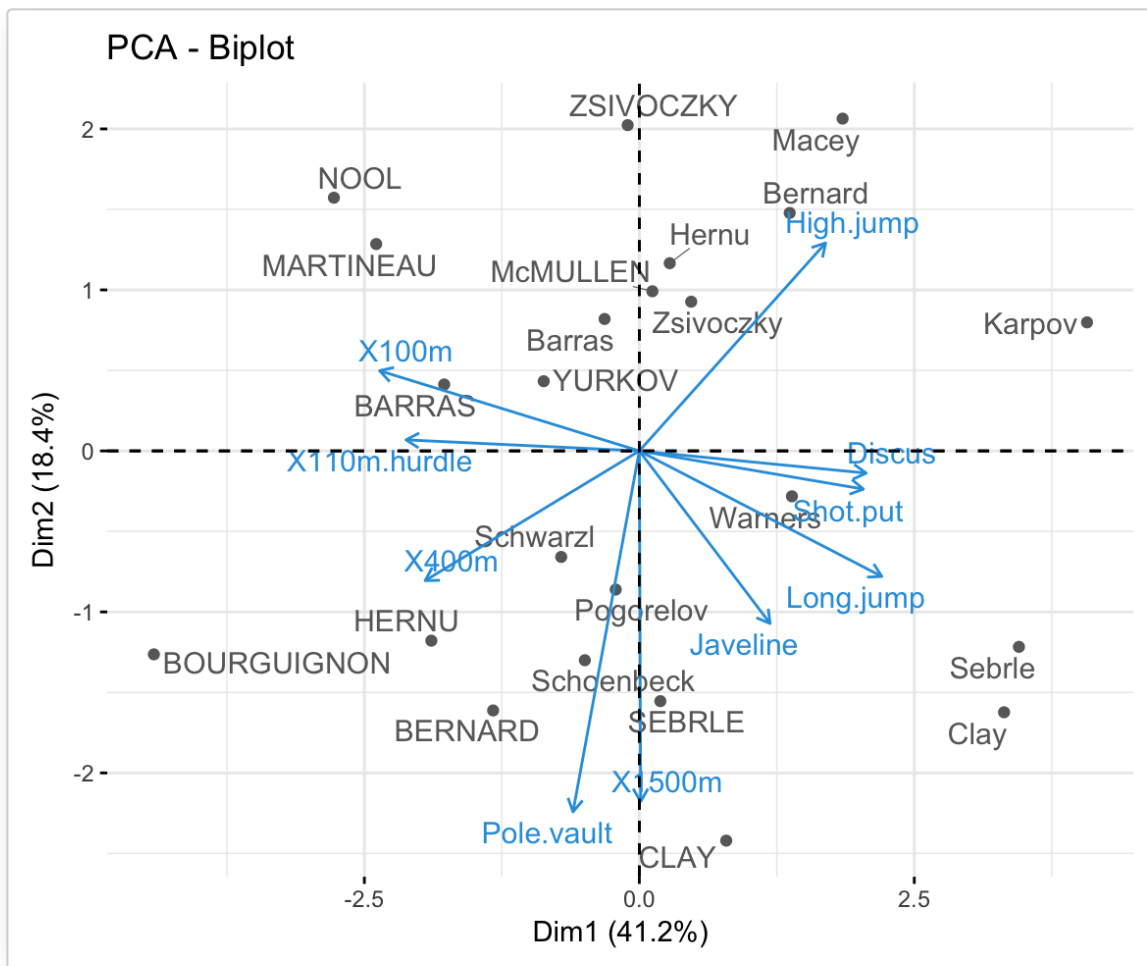
5. Graph of variables. Positive correlated variables point to the same side of the plot. Negative correlated variables point to opposite sides of the graph.

```
fviz_pca_var(res.pca,
  col.var = "contrib", # Color by contributions to the PC
  gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"),
  repel = TRUE        # Avoid text overlapping
)
```



6. Biplot of individuals and variables

```
fviz_pca_biplot(res.pca, repel = TRUE,  
  col.var = "#2E9FDF", # Variables color  
  col.ind = "#696969" # Individuals color  
)
```



Access to the PCA results

```
library(factoextra)
# Eigenvalues
eig.val <- get_eigenvalue(res.pca)
eig.val

# Results for Variables
res.var <- get_pca_var(res.pca)
res.var$coord      # Coordinates
res.var$contrib     # Contributions to the PCs
res.var$cos2       # Quality of representation
# Results for individuals
res.ind <- get_pca_ind(res.pca)
res.ind$coord      # Coordinates
res.ind$contrib     # Contributions to the PCs
res.ind$cos2       # Quality of representation
```

Predict using PCA

In this section, we'll show how to predict the coordinates of supplementary individuals and variables using only the information provided by the previously performed PCA.

Supplementary individuals

1. Data: rows 24 to 27 and columns 1 to 10 [in decathlon2 data sets]. The new data must contain columns (variables) with the same names and in the same order as the active data used to compute PCA.

```
# Data for the supplementary individuals
ind.sup <- decathlon2[24:27, 1:10]
ind.sup[, 1:6]
```

```
##           X100m Long.jump Shot.put High.jump X400m X110m.hurdle
## KARPOV    11.0      7.30     14.8      2.04  48.4         14.1
## WARNERS   11.1      7.60     14.3      1.98  48.7         14.2
## Nool      10.8      7.53     14.3      1.88  48.8         14.8
## Drews     10.9      7.38     13.1      1.88  48.5         14.0
```

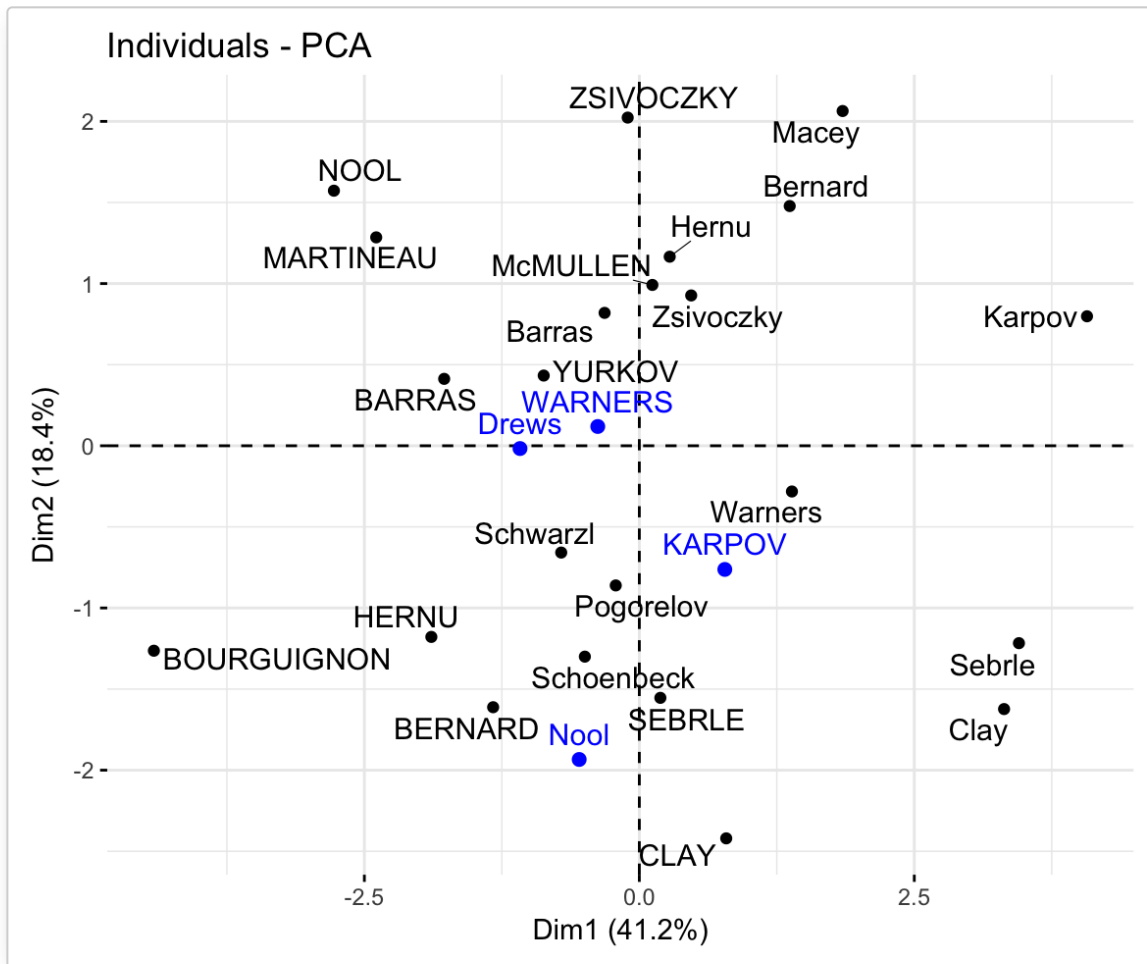
2. Predict the coordinates of new individuals data. Use the R base function *predict()*:

```
ind.sup.coord <- predict(res.pca, newdata = ind.sup)
ind.sup.coord[, 1:4]
```

```
##           PC1      PC2      PC3      PC4
## KARPOV    0.777 -0.762  1.597  1.686
## WARNERS  -0.378  0.119  1.701 -0.691
## Nool      -0.547 -1.934  0.472 -2.228
## Drews     -1.085 -0.017  2.982 -1.501
```

3. Graph of individuals including the supplementary individuals:

```
# Plot of active individuals
p <- fviz_pca_ind(res.pca, repel = TRUE)
# Add supplementary individuals
fviz_add(p, ind.sup.coord, color = "blue")
```



The predicted coordinates of individuals can be manually calculated as follow:

1. Center and scale the new individuals data using the center and the scale of the PCA
2. Calculate the predicted coordinates by multiplying the scaled values with the eigenvectors (loadings) of the principal components.

The R code below can be used :

```
# Centering and scaling the supplementary individuals
ind.scaled <- scale(ind.sup,
                    center = res.pca$center,
                    scale = res.pca$scale)

# Coordinates of the individuals
coord_func <- function(ind, loadings){
  r <- loadings*ind
  apply(r, 2, sum)
}

pca.loadings <- res.pca$rotation
ind.sup.coord <- t(apply(ind.scaled, 1, coord_func, pca.loadings ))
ind.sup.coord[, 1:4]
```

```
##          PC1    PC2    PC3    PC4
## KARPOV   0.777 -0.762  1.597  1.686
## WARNERS -0.378  0.119  1.701 -0.691
## Nool    -0.547 -1.934  0.472 -2.228
## Drews   -1.085 -0.017  2.982 -1.501
```

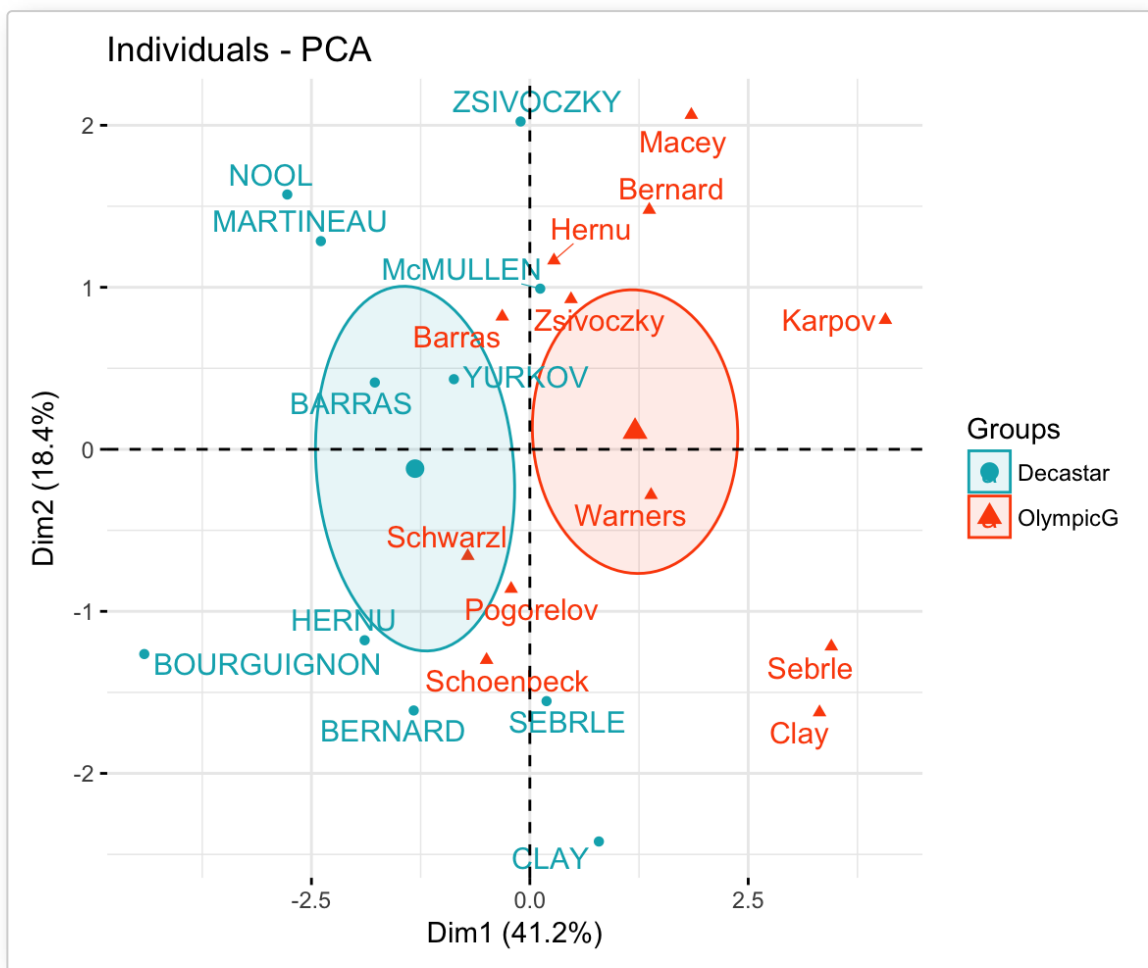
Supplementary variables

Qualitative / categorical variables

The data sets `decathlon2` contain a *supplementary qualitative variable* at columns 13 corresponding to the type of competitions.

Qualitative / categorical variables can be used to color individuals by groups. The grouping variable should be of same length as the number of active individuals (here 23).

```
groups <- as.factor(decathlon2$Competition[1:23])
fviz_pca_ind(res.pca,
  col.ind = groups, # color by groups
  palette = c("#00AFBB", "#FC4E07"),
  addEllipses = TRUE, # Concentration ellipses
  ellipse.type = "confidence",
  legend.title = "Groups",
  repel = TRUE
)
```



Calculate the coordinates for the levels of grouping variables. The coordinates for a given group is calculated as the mean coordinates of the individuals in the group.

```
library(magrittr) # for pipe %>%
library(dplyr)    # everything else
```

```
# 1. Individual coordinates
res.ind <- get_pca_ind(res.pca)
# 2. Coordinate of groups
coord.groups <- res.ind$coord %>%
  as_data_frame() %>%
  select(Dim.1, Dim.2) %>%
  mutate(competition = groups) %>%
  group_by(competition) %>%
  summarise(
    Dim.1 = mean(Dim.1),
    Dim.2 = mean(Dim.2)
  )
coord.groups
```

```
## # A tibble: 2 x 3
##   competition Dim.1 Dim.2
##
## 1   Decastar -1.31 -0.119
## 2   OlympicG  1.20  0.109
```

Quantitative variables

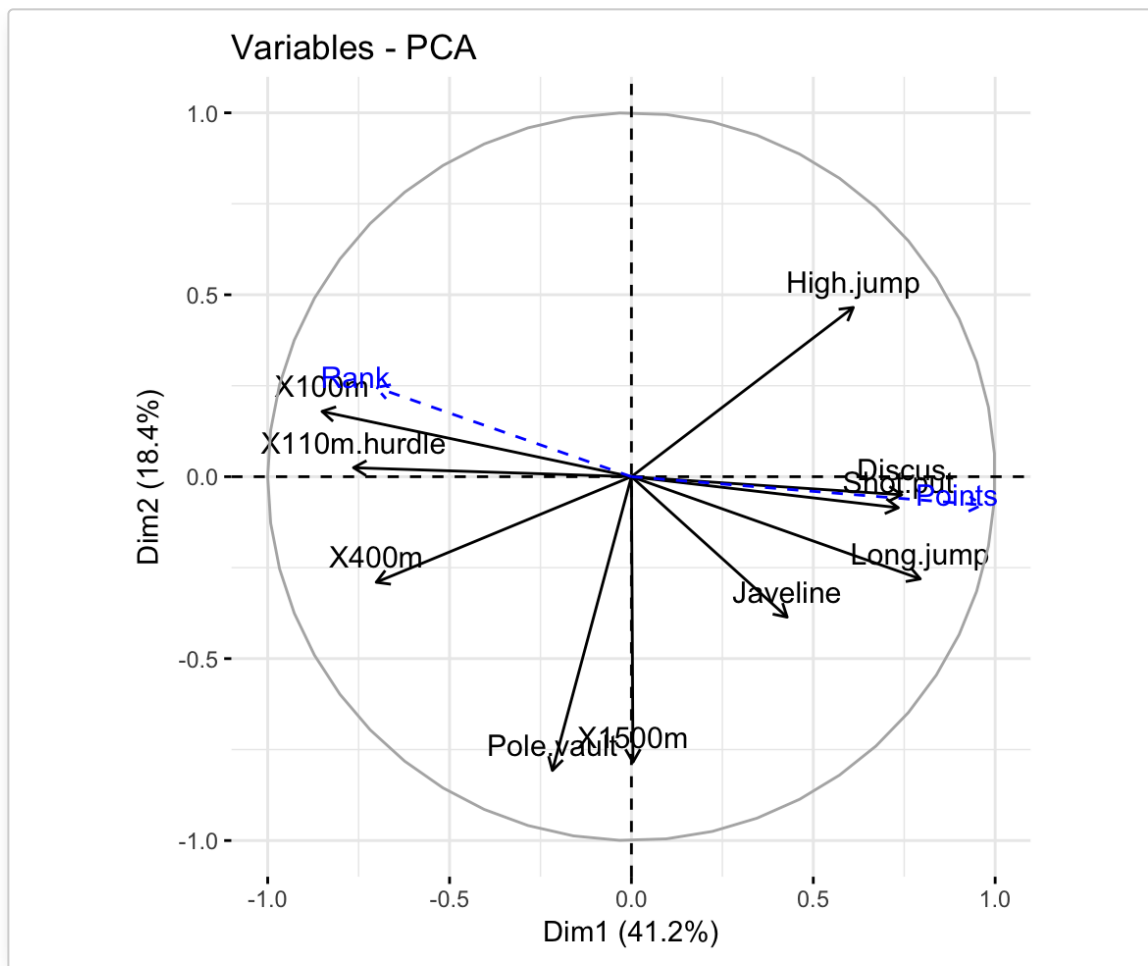
Data: columns 11:12. Should be of same length as the number of active individuals (here 23)

```
quanti.sup <- decathlon2[1:23, 11:12, drop = FALSE]
head(quanti.sup)
```

```
##           Rank Points
## SEBRLE      1   8217
## CLAY        2   8122
## BERNARD     4   8067
## YURKOV      5   8036
## ZSIVOCZKY   7   8004
## McMULLEN    8   7995
```

The coordinates of a given quantitative variable are calculated as the correlation between the quantitative variables and the principal components.

```
# Predict coordinates and compute cos2
quanti.coord <- cor(quanti.sup, res.pca$x)
quanti.cos2 <- quanti.coord^2
# Graph of variables including supplementary variables
p <- fviz_pca_var(res.pca)
fviz_add(p, quanti.coord, color = "blue", geom = "arrow")
```



Theory behind PCA results

PCA results for variables

Here we'll show how to calculate the PCA results for variables: coordinates, cos2 and contributions:

- **var.coord** = loadings * the component standard deviations
- **var.cos2** = var.coord^2
- **var.contrib**. The contribution of a variable to a given principal component is (in percentage) : $(\text{var.cos2} * 100) / (\text{total cos2 of the component})$

```
# Helper function
#::::::::::::::::::::::::::::::::::::
var_coord_func <- function(loadings, comp.sdev){
  loadings*comp.sdev
}
# Compute Coordinates
#::::::::::::::::::::::::::::::::::::
loadings <- res.pca$rotation
sdev <- res.pca$sdev
var.coord <- t(apply(loadings, 1, var_coord_func, sdev))
head(var.coord[, 1:4])
```

```
##          PC1      PC2      PC3      PC4
## X100m    -0.851  0.1794 -0.302  0.0336
## Long.jump  0.794 -0.2809  0.191 -0.1154
## Shot.put  0.734 -0.0854 -0.518  0.1285
## High.jump  0.610  0.4652 -0.330  0.1446
## X400m    -0.702 -0.2902 -0.284  0.4308
## X110m.hurdle -0.764  0.0247 -0.449 -0.0169
```

```
# Compute Cos2
#::::::::::::::::::::::::::::::::::::
var.cos2 <- var.coord^2
head(var.cos2[, 1:4])
```

```
##          PC1      PC2      PC3      PC4
## X100m    0.724 0.032184 0.0909 0.001127
## Long.jump 0.631 0.078881 0.0363 0.013315
## Shot.put  0.539 0.007294 0.2679 0.016504
## High.jump 0.372 0.216424 0.1090 0.020895
## X400m    0.492 0.084203 0.0804 0.185611
## X110m.hurdle 0.584 0.000612 0.2015 0.000285
```

```
# Compute contributions
#::::::::::::::::::::::::::::::::::::
comp.cos2 <- apply(var.cos2, 2, sum)
contrib <- function(var.cos2, comp.cos2){var.cos2*100/comp.cos2}
var.contrib <- t(apply(var.cos2,1, contrib, comp.cos2))
head(var.contrib[, 1:4])
```

```
##          PC1      PC2      PC3      PC4
## X100m    17.54  1.7505  7.34  0.1376
## Long.jump 15.29  4.2904  2.93  1.6249
## Shot.put  13.06  0.3967 21.62  2.0141
## High.jump  9.02 11.7716  8.79  2.5499
## X400m    11.94  4.5799  6.49 22.6509
## X110m.hurdle 14.16  0.0333 16.26  0.0348
```

PCA results for individuals

- `ind.coord` = `res.pca$x`
- Cos2 of individuals. Two steps:
 - Calculate the square distance between each individual and the PCA center of gravity: $d2 = [(var1_ind_i - mean_var1)/sd_var1]^2 + \dots + [(var10_ind_i - mean_var10)/sd_var10]^2 + \dots$
 - Calculate the cos2 as $ind.coord^2/d2$
- Contributions of individuals to the principal components: $100 * (1 / number_of_individuals) * (ind.coord^2 / comp_sdev^2)$. Note that the sum of all the contributions per column is 100

```
# Coordinates of individuals
#::::::::::::::::::::::::::::::::::::
```

```
ind.coord <- res.pca$x
head(ind.coord[, 1:4])
```

```
##           PC1    PC2    PC3    PC4
## SEBRLE    0.191 -1.554 -0.628  0.0821
## CLAY      0.790 -2.420  1.357  1.2698
## BERNARD   -1.329 -1.612 -0.196 -1.9209
## YURKOV    -0.869  0.433 -2.474  0.6972
## ZSIVOCZKY -0.106  2.023  1.305 -0.0993
## McMULLEN  0.119  0.992  0.844  1.3122
```

```
# Cos2 of individuals
#::::::::::::::::::::::::::::::::::
# 1. square of the distance between an individual and the
# PCA center of gravity
center <- res.pca$center
scale<- res.pca$scale
getdistance <- function(ind_row, center, scale){
  return(sum(((ind_row-center)/scale)^2))
}
d2 <- apply(decathlon2.active,1,getdistance, center, scale)
# 2. Compute the cos2. The sum of each row is 1
cos2 <- function(ind.coord, d2){return(ind.coord^2/d2)}
ind.cos2 <- apply(ind.coord, 2, cos2, d2)
head(ind.cos2[, 1:4])
```

```
##           PC1    PC2    PC3    PC4
## SEBRLE    0.00753 0.4975 0.08133 0.00139
## CLAY      0.04870 0.4570 0.14363 0.12579
## BERNARD   0.19720 0.2900 0.00429 0.41182
## YURKOV    0.09611 0.0238 0.77823 0.06181
## ZSIVOCZKY 0.00157 0.5764 0.23975 0.00139
## McMULLEN  0.00218 0.1522 0.11014 0.26649
```

```
# Contributions of individuals
#::::::::::::::::::::::::::::::::::
contrib <- function(ind.coord, comp.sdev, n.ind){
  100*(1/n.ind)*ind.coord^2/comp.sdev^2
}
ind.contrib <- t(apply(ind.coord, 1, contrib,
                      res.pca$sdev, nrow(ind.coord)))
head(ind.contrib[, 1:4])
```

```
##           PC1    PC2    PC3    PC4
## SEBRLE    0.0385  5.712  1.385  0.0357
## CLAY      0.6581 13.854  6.460  8.5557
## BERNARD   1.8627  6.144  0.135 19.5783
## YURKOV    0.7969  0.443 21.476  2.5794
```

ZSIVOCZKY 0.0118 9.682 5.975 0.0523
 ## McMULLEN 0.0148 2.325 2.497 9.1353

Last update : 08/10/2017

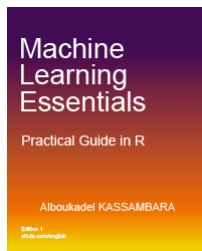
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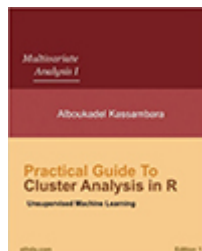
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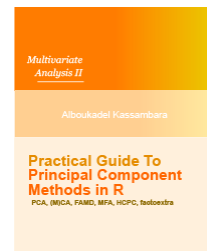
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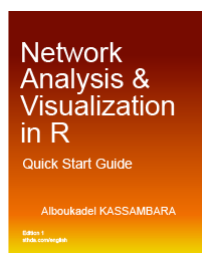
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Alam 11/11/2018 at 12h13
Visitor

Thank you very much for this nice tutorial.

I have one problem. How to italicize the variable name in PCA correlation circle plot.

I am looking forward to hearing.

#642



Mike 10/18/2018 at 09h57
Visitor

Sorry to Necro this thread, but I have to say, what a fantastic guide! It has come in very helpful. Thank you so much for putting this together. I'm curious if anyone else has had trouble plotting the ellipses?

When I try to run the code under the "Qualitative / categorical variables" section I am returned with this error:

```
<Computation failed in `stat_conf_ellipse()` : missing value where TRUE/FALSE needed>
```

I looked up Stat_conf_ellipse to learn more about it, loaded ggpubr, and added it to my command. After running it, the plot appears with the correct groupings but no ellipses, along with the following error:

```
<Error in .check_axes(axes, .length = 2) : axes should be of length 2>
```

My plot scale is 2 so this makes sense, the length of the axes needs to fit in the plot, so less than 2. I change this and retry, and then I get <Error in check_axes(axes, .length = 0.5) : could not find function "check_axes",>.

I have tried numerous combinations using "stat_conf_ellipse" and none of them have worked. I nested it in the fviz_pca_ind command, added it on the end with a +, add and remove functions from the stat_conf_ellipse help page.....nothing I try is working.

Does anyone have experience with this and thoughts on why it might be failing? Again, it plots fine with proper groups and colors, but no ellipses. Here was the last iteration of code I had:

```
fviz_pca_ind(mydata.pca, col.ind = groups, palette = c("#00AFBB", "#FC4E07", "#bb00a8"), addEllipses = TRUE, ellipse.type = "confidence", legend.title = "Groups", repel = TRUE, stat_conf_ellipse(position = "identity", na.rm = FALSE, show.legend = NA, inherit.aes = true, level = 0.95, npoint = 100, bary = true))
```

The error on the above code: Error in .check_axes(axes, .length = 2) : axes should be of length 2

Thanks for any help!

#633



Konig 11/19/2017 at 17h46
Visitor

Hi there,

Could you help me out interpreting the correlation of Rank and Points against the PCs?
Is there a way to determine whether these are statistically significant to the PCA results?
Thanks!

#303



Visitor 11/07/2017 at 19h13
Visitor

Want to learn about PCA

#289

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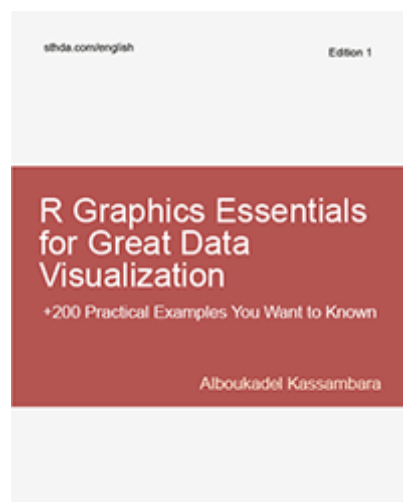
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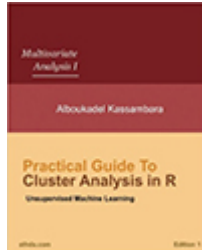
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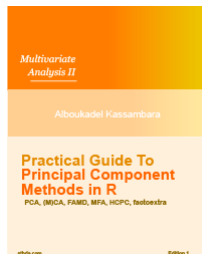
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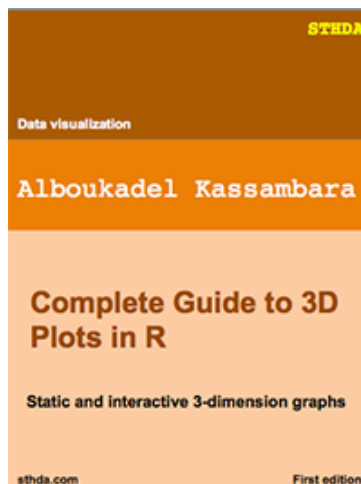
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