# Package: plsdepot (via r-universe)

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```
Type Package
Title Partial Least Squares (PLS) Data Analysis Methods
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Description Different methods for PLS analysis of one or two data
      tables such as Tucker's Inter-Battery, NIPALS, SIMPLS,
      SIMPLS-CA, PLS Regression, and PLS Canonical Analysis. The main
      reference for this software is the awesome book (in French) 'La
      Regression PLS: Theorie et Pratique' by Michel Tenenhaus.
Depends R (>= 2.15.1)
Suggests FactoMineR
License GPL-3
LazyLoad yes
Collate 'nipals.R' 'plot.nipals.R' 'plot.plsca.R' 'plot.plsreg1.R'
      'plot.plsreg2.R' 'plsca.R' 'plsreg1.R' 'plsreg2.R'
      'print.nipals.R' 'print.plsca.R' 'print.plsreg1.R'
      'print.plsreg2.R' 'interbat.R' 'plot.interbat.R'
      'print.interbat.R' 'print.simpls.R' 'print.simplsca.R'
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```

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# Description

Data set with six variables measured on 24 cars (no missing values)

## Usage

data(carscomplete)

## **Format**

A data frame with 6 variables measured on the 24 cars.

Num	Variable	Description
1	Cylindree	Engine
2	Puissance	Power
3	Vitese	Speed
4	Poids	Weight
5	Longueur	Length
6	Largeur	Height

carsmissing 3

## **Details**

This is data with no missing values

#### Source

Tenenhaus M. (1998) La Regression PLS: theorie et pratique. Table 4, page 67

## References

Tenenhaus M. (1998) La Regression PLS: theorie et pratique Paris: Editions Technip

## **Examples**

```
data(carscomplete)
head(carscomplete)
```

carsmissing

carsmissing data set

## **Description**

Data set with six variables measured on 24 cars

## Usage

data(carsmissing)

#### **Format**

A data frame with 6 variables measured on the 24 cars (contains missing values).

Num	Variable	Description
1	Cylindree	Engine
2	Puissance	Power
3	Vitese	Speed
4	Poids	Weight
5	Longueur	Length
6	Largeur	Height

## **Details**

This is data contains one missing value in each row

## Source

Tenenhaus M. (1998) La Regression PLS: theorie et pratique. Table 5, page 69

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#### References

Tenenhaus M. (1998) La Regression PLS: theorie et pratique Paris: Editions Technip

## **Examples**

```
data(carsmissing)
head(carsmissing)
```

cornell

Cornell data set

## Description

Data describing the composition of 12 octane mixtures (units measured in proportions)

## Usage

```
data(cornell)
```

#### **Format**

A data frame with 12 observations on the following 8 variables.

Num	Variable	Description
1	Distillation	Direct Distillation
2	Reformed	Reformed
3	NaphthaTher	Thermal cracking Naphtha
4	NaphthaCat	Catalytic cracking Naphtha
5	Polymer	Polymer
6	Alkylat	Alkylat
7	NatEssence	Natural Essence
8	Octane	Octane

## Source

```
Tenenhaus M. (1998) Table 6, page 78
```

#### References

Tenenhaus M. (1998) La Regression PLS: theorie et pratique Paris: Editions Technip

```
data(cornell)
head(cornell)
```

interbat 5

interbat	Tucker's Inter-Battery Method of Factor Analysis	
	·	

## Description

The function interbat performs Tucker's Inter-Battery method of factor analysis as described in Michel Tenenhaus book *La Regression PLS*, chapter 3

## Usage

```
interbat(X, Y, scaled = TRUE)
```

## Arguments

Χ	Numeric matrix or data frame with two or more columns (X-block).
Υ	Numeric matrix or data frame with two or more columns (Y-block).
scaled	Logical value indicating whether to scale the data (TRUE by default).

#### **Details**

Arguments X and Y must contain more than one variable. No missing data are allowed.

## Value

An object of class "interbat", basically a list with the following elements:

values	The extracted eigenvalues
x.scores	scores of the X-block (also known as T components)
x.wgs	weights of the X-block
y.scores	scores of the Y-block (also known as U components)
y.wgs	weights of the Y-block
cor.xt	correlations between X and T
cor.yu	correlations between Y and U
cor.xu	correlations between X and U
cor.yt	correlations between Y and T
cor.tu	correlations between T and U
R2X	explained variance of X by T
R2Y	explained variance of Y by U
com.xu	communality of X with U
com.yt	communality of Y with T
statistic	Phi statistic values for assessing the number of relevant components

6 linnerud

#### Author(s)

Gaston Sanchez

#### References

```
Tenenhaus, M. (1998) La Regression PLS. Theorie et Pratique. Paris: Editions TECHNIP. Tucker, L.R. (1958) An inter-battery method of factor analysis. Psychometrika, 23(2): 111-136.
```

#### See Also

```
plot.interbat, plsca
```

## **Examples**

```
## Not run:
# load data linnerud
data(linnerud)

# apply inter-battery method
ib = interbat(linnerud[,1:3], linnerud[,4:6])

# plot variables
plot(ib, what="variables")

# plot observations
plot(ib, what="observations", comps=c(1,1), where=c("t","u"))
## End(Not run)
```

linnerud

Linnerud data set

#### **Description**

Thris data set contains three physiological and three exercise variables measured on 20 men

#### Usage

```
data(linnerud)
```

#### **Format**

A data frame with 20 observations on the following 6 variables.

Num	Variable	Description
1	Weight	Weight
2	Waist	Waist size
3	Pulse	Pulse

nipals 7

4	Pulls	Pull-ups
5	Squats	Squats
6	Jumps	Jumps

#### **Source**

```
Tenenhaus M. (1998) Table 1, page 15
```

#### References

Tenenhaus M. (1998) La Regression PLS: theorie et pratique Paris: Editions Technip

## **Examples**

```
data(linnerud)
head(linnerud)
```

nipals

NIPALS: Non-linear Iterative Partial Least Squares

## Description

Principal Components Analysis with NIPALS algorithm

## Usage

```
nipals(Data, comps = 2, scaled = TRUE)
```

## **Arguments**

Data A numeric matrix or data frame (which may contain missing values).

comps Number of components to be calculated (by default 2)

scaled A logical value indicating whether to scale the data (TRUE by default).

#### **Details**

The function nipals performs Principal Components Analysis of a data matrix that may contain missing values.

8 nipals

#### Value

An object of class "nipals", basically a list with the following elements:

When the analyzed data contain missing values, the help interpretation tools (e.g. cor.xt, disto, contrib, cos, dmod) may not be meaningful, that is to say, some of the results may not be coherent.

values The pseudo eigenvalues

scores The extracted scores (i.e. components)

loadings The loadings

cor.xt Correlations between the variables and the scores disto Squared distance of the observations to the origin

contrib Contributions of the observations (rows)

cos Squared cosinus

dmod Distance to the Model

#### Author(s)

Gaston Sanchez

#### References

```
Tenenhaus, M. (1998) La Regression PLS. Theorie et Pratique. Paris: Editions TECHNIP. Tenenhaus, M. (2007) Statistique. Methodes pour decrire, expliquer et prevoir. Paris: Dunod.
```

#### See Also

```
plot.nipals, plsreg1
```

```
## Not run:
    # load datasets carscomplete and carsmissing
    data(carscomplete) # complete data
    data(carsmissing) # missing values

# apply nipals
    my_nipals1 = nipals(carscomplete)
    my_nipals2 = nipals(carsmissing)

# plot variables (circle of correlations)
    plot(my_nipals1, what="variables", main="Complete data")
    plot(my_nipals2, what="variables", main="Missing data")

# plot observations with labels
    plot(my_nipals1, what="observations", show.names=TRUE, main="Complete data")
    plot(my_nipals2, what="observations", show.names=TRUE, main="Missing data")

# compare results between my_nipals1 and my_nipals2
```

plot.interbat 9

plot.interbat

Plot inter-battery basic results

## **Description**

Plot method for objects of class "interbat". This function plots either the variables or the observations, on the selected components (i.e. scores). Variables are plotted inside the circle of correlations. Observations are plotted on a scatter plot.

#### Usage

```
## S3 method for class 'interbat'
plot(x, what = "variables",
   comps = c(1, 2), where = c("t", "t"), cex = 1,
   col.xlabels = "#5592e3", col.ylabels = "#e3a654",
   yfont = 1, pos = NULL, offset = 0.1,
   col.xarrows = "#5b9cf255", col.yarrows = "#e3a65455",
   lwd = 3, length = 0, angle = 0, col.points = "#5592e3",
   pch = 21, pt.bg = "#5b9cf255", show.names = FALSE,
   xpd = TRUE, xlab = NULL, ylab = NULL, main = NULL,
   col.main = "gray35", cex.main = 1.2,
   col.axis = "gray40", show.grid = TRUE,
   col.grid = "gray95", ...)
```

## **Arguments**

X	An object of class "interbat".
what	What to plot. Options are "variables" and "observations".
comps	An integer vector of length two to indicate which components to plot.
where	Where to plot the observations. A character vector of length two to indicate which components to use when plotting observations. This parameter will take into account the values in comps. Possible options are: $c("t","u")$ for using x-y components, $c("t","t")$ , for using x components, and $c("u","u")$ for using y components. Default $c("t","t")$ .
cex	Character expansion for labels and points.
col.xlabels	Color for labels of X-block variables.
col.ylabels	Color for labels of Y-block variables.

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yfont Integer for specifying which font to use for Y-block labels. See font in graphical

parameters par.

pos Position for the text (see graphical paramaters par)

offset When pos is specified, this value gives the offset of the labels.

col.xarrows Color for the X-block arrows.

col.yarrows Color for the Y-block arrows.

1wd The line width of arrows.

length Length of the edges of the arrow head (in inches).

angle Angle from the shaft of the arrow to the edge of the arrow head.

col.points Color for the points when what="observations".

pch Plotting character symbol to use (see par).

pt.bg Background (fill) color for the points given by pch=21:25.

show.names Logical indicating whether to show labels of points. Only used when what="observations"

xpd Logical for controlling clipping region of names and labels.

xlab A title for the x axis.

ylab A title for the y axis.

main Main title of the plot.

col.main Color of main title.

cex.main Character expansion of main title.

col.axis Color of axis annotations (tick marks and labels). show.grid Logical indicating whether to show grid lines.

col.grid Color of grid lines. Only used when show.grid=TRUE.

... Further arguments are passed to labels or points.

#### **Details**

Variables are displayed using the correlations of each block of variables with the components of the other block: \$cor.xu-vs-\$cor.yt.

#### Author(s)

Gaston Sanchez

#### See Also

interbat

plot.nipals 11

#### **Examples**

```
# load dataset linnerud
data(linnerud)
# apply nipals
ib = interbat(linnerud[,1:3], linnerud[,4:6])
# plot variables (circle of correlations)
plot(ib, what="variables")
# plot observations (as points) using components (t1,u1)
plot(ib, what="observations", comps=c(1,1), where=c("t","u"))
# plot observations with names using components (t1,u1)
plot(ib, what="observations", comps=c(1,1),
     where=c("t","u"), show.names=TRUE)
# plot observations (as points) using components (t1,t2)
plot(ib, what="observations", comps=c(1,2), where=c("t","t"))
# plot observations (as points) using components (u1,u2)
plot(ib, what="observations", comps=c(1,2), where=c("u","u"))
## End(Not run)
```

plot.nipals

Plot NIPALS basic results

#### **Description**

Plot method for objects of class "nipals". This function plots either the variables or the observations, on the selected components (i.e. scores). Variables are plotted inside the circle of correlations. Observations are plotted on a scatter plot.

## Usage

```
## S3 method for class 'nipals'
plot(x, what = "variables",
   comps = c(1, 2), cex = 1, col.labels = "#5592e3",
   pos = NULL, offset = 0.1, col.arrows = "#5b9cf255",
   lwd = 3.5, length = 0, angle = 0,
   col.points = "#5592e3", pch = 21, pt.bg = "#5b9cf255",
   show.names = FALSE, xpd = TRUE, xlab = NULL,
   ylab = NULL, main = NULL, col.main = "gray35",
   cex.main = 1.2, col.axis = "gray40", show.grid = TRUE,
   col.grid = "gray95", ...)
```

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#### **Arguments**

x An object of class "nipals".

what What to plot. Options are "variables" and "observations"

comps An integer vector of length two to indicate which components to plot

cex Character expansion for labels and points.

col.labels Color for labels of variables.

pos Position for the labels text (see par).

offset When pos is specified, this value gives the offset of the labels.

col. arrows Color for the arrows when plotting variables.

1wd The line width of arrows.

length Length of the edges of the arrow head (in inches).

angle Angle from the shaft of the arrow to the edge of the arrow head.

col.points Color for the points when what="observations".

pch Plotting character symbol to use (see par).

pt.bg Background (fill) color for the points given by pch=21:25.

show. names Logical indicating whether to show names of points. Only used when what="observations"

xpd Logical for controlling clipping region of labels and names.

xlab Title for the x axis.
ylab Title for the y axis.
main Main title of the plot.
col.main Color of main title.

cex.main Character expansion of main title.

col.axis Color of axis annotations (tick marks and labels). show.grid Logical indicating whether to show grid lines.

col.grid Color of grid lines. Only used when show.grid=TRUE.

... Further arguments are passed to labels or points.

#### **Details**

Variables are displayed using the correlations in \$cor.xt.

#### Author(s)

Gaston Sanchez

#### See Also

nipals

plot.plsca 13

#### **Examples**

```
## Not run:
# load data climbing ropes
data(ropes)

# apply nipals with 3 components
nip1 = nipals(ropes[,-1], comps=3)

# plot variables (correlations)
plot(nip1)

# plot observations
plot(nip1, what="obs")

# plot observations with names
plot(nip1, what="obs", show.names=TRUE)

## End(Not run)
```

plot.plsca

Plot PLS-CA basic results

#### **Description**

Plot method for objects of class "plsca". This function plots either the variables or the observations, on the selected components (i.e. scores). Variables are plotted inside the circle of correlations. Observations are plotted on a scatter plot.

## Usage

```
## S3 method for class 'plsca'
plot(x, what = "variables",
   comps = c(1, 2), where = c("t", "t"), cex = 1,
   col.xlabels = "#5592e3", col.ylabels = "#fe9429",
   yfont = 2, pos = NULL, offset = 0.1,
   col.xarrows = "#5b9cf255", col.yarrows = "#fe942955",
   lwd = 3, length = 0, angle = 0, col.points = "#5592e3",
   pch = 21, pt.bg = "#5b9cf255", show.names = FALSE,
   xpd = TRUE, xlab = NULL, ylab = NULL, main = NULL,
   col.main = "gray35", cex.main = 1.2,
   col.axis = "gray40", show.grid = TRUE,
   col.grid = "gray95", ...)
```

#### **Arguments**

x An object of class "plsca".
 what What to plot. Options are "variables" and "observations".
 comps An integer vector of length two to indicate which components to plot.

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where Where to plot the observations. A character vector of length two to indicate

which components to use when plotting observations. This parameter will take into account the values in comps. Possible options are: c("t", "u") for using x-y components, c("t", "t"), for using x components, and c("u", "u") for using

y components. Default c("t", "t").

cex Character expansion for labels and points.

col.xlabels Color for labels of X-block variables.
col.ylabels Color for labels of Y-block variables.

yfont Integer for specifying which font to use for Y-block labels. See font in graphical

parameters par.

pos Position for the text (see graphical paramaters par).

offset When pos is specified, this value gives the offset of the labels.

col.xarrows Color for the X-block arrows.

col.yarrows Color for the Y-block arrows.

The line width of arrows.

length Length of the edges of the arrow head (in inches).

angle Angle from the shaft of the arrow to the edge of the arrow head.

col.points Color for the points when what="observations".

pch Plotting character symbol to use (see par).

pt.bg Background (fill) color for the points given by pch=21:25.

show.names Logical indicating whether to show labels of points. Only used when what="observations".

xpd Logical for controlling clipping region of names and labels.

xlab A title for the x axis.
ylab A title for the y axis.
main Main title of the plot.
col.main Color of main title.

cex.main Character expansion of main title.

col.axis Color of axis annotations (tick marks and labels). show.grid Logical indicating whether to show grid lines.

col.grid Color of grid lines. Only used when show.grid=TRUE.

... Further arguments are passed to labels or points.

#### Details

Variables are displayed using the correlations of each block of variables with its set of components: \$cor.xt and \$cor.yu.

#### Author(s)

Gaston Sanchez

#### See Also

plsca

#### **Examples**

```
## Not run:
# load dataset linnerud
 data(linnerud)
 # apply plsca
 my_plsca = plsca(linnerud[,1:3], linnerud[,4:6])
 # plot variables (circle of correlations)
 plot(my_plsca, what="variables")
 # plot observations (as points) using components (t1,u1)
 plot(my_plsca, what="observations", comps=c(1,1), where=c("t","u"))
 # plot observations with names using components (t1,u1)
 plot(my_plsca, what="observations", comps=c(1,1),
      where=c("t","u"), show.names=TRUE)
 # plot observations (as points) using components (t1,t2)
 plot(my_plsca, what="observations", comps=c(1,2), where=c("t","t"))
 # plot observations (as points) using components (u1,u2)
 plot(my_plsca, what="observations", comps=c(1,2), where=c("u","u"))
## End(Not run)
```

plot.plsreg1

Plot PLS-R1 basic results

## **Description**

Plot method for objects of class "plsreg1". This function plots either the variables or the observations, on the selected components (i.e. scores). Variables are plotted inside the circle of correlations. Observations are plotted on a scatter plot.

## Usage

```
## S3 method for class 'plsreg1'
plot(x, what = "variables",
   comps = c(1, 2), where = c("t", "t"), cex = 1,
   col.xlabels = "#5592e3", col.ylabel = "#fe9429",
   yfont = 2, pos = NULL, offset = 0.1,
   col.xarrows = "#5b9cf255", col.yarrows = "#fe942955",
   lwd = 3, length = 0, angle = 0, col.points = "#5592e3",
   pch = 21, pt.bg = "#5b9cf255", show.names = FALSE,
```

```
xpd = TRUE, xlab = NULL, ylab = NULL, main = NULL,
col.main = "gray35", cex.main = 1.2,
col.axis = "gray40", show.grid = TRUE,
col.grid = "gray95", ...)
```

#### **Arguments**

x An object of class "plsreg1".

what What to plot. Options are "variables" and "observations".

comps An integer vector of length two to indicate which components to plot.

where Where to plot the observations. A character vector of length two to indicate

which components to use when plotting observations. This parameter will take into account the values in comps. Possible options are: c("t", "u") for using x-y components, c("t", "t"), for using x components, and c("u", "u") for using

y components. Default c("t", "t").

cex Character expansion for labels and points.

col.xlabels Color for labels of X-block variables.
col.ylabel Color for labels of Y-block variables.

yfont Integer for specifying which font to use for Y-block labels. See font in graphical

parameters par.

pos Position for the text (see graphical paramaters par).

offset When pos is specified, this value gives the offset of the labels.

col.xarrows Color for the X-block arrows.
col.yarrows Color for the Y-block arrows.
lwd The line width of arrows.

length Length of the edges of the arrow head (in inches).

angle Angle from the shaft of the arrow to the edge of the arrow head.

col.points Color for the points when what="observations".

pch Plotting character symbol to use (see par).

pt.bg Background (fill) color for the points given by pch=21:25.

show.names Logical indicating whether to show labels of points. Only used when what="observations".

xpd Logical for controlling clipping region of names and labels.

xlab A title for the x axis.
ylab A title for the y axis.
main Main title of the plot.
col.main Color of main title.

cex.main Character expansion of main title.

col.axis Color of axis annotations (tick marks and labels). show.grid Logical indicating whether to show grid lines.

col.grid Color of grid lines. Only used when show.grid=TRUE.

Further arguments are passed to labels or points.

#### **Details**

Variables are displayed using the correlations in \$cor.xyt.

#### Author(s)

Gaston Sanchez

#### See Also

plsreg1

#### **Examples**

```
## Not run:
# load dataset cornell
data(cornell)
 # apply plsreg1
 myplsr1 = plsreg1(cornell[,1:7], cornell[,8,drop=FALSE])
 # plot variables (circle of correlations)
 plot(myplsr1, what="variables")
 # plot observations (as points) using components (t1,u1)
 plot(myplsr1, what="observations", comps=c(1,1), where=c("t","u"))
 # plot observations with names using components (t1,u1)
 plot(myplsr1, what="observations", comps=c(1,1),
     where=c("t","u"), show.names=TRUE)
 # plot observations (as points) using components (t1,t2)
 plot(myplsr1, what="observations", comps=c(1,2), where=c("t","t"))
 # plot observations (as points) using components (u1,u2)
 plot(myplsr1, what="observations", comps=c(1,2), where=c("u","u"))
## End(Not run)
```

plot.plsreg2

Plot PLS-R2 basic results

## **Description**

Plot method for objects of class "plsreg2". This function plots either the variables or the observations, on the selected components (i.e. scores). Variables are plotted inside the circle of correlations. Observations are plotted on a scatter plot.

#### **Usage**

```
## S3 method for class 'plsreg2'
plot(x, what = "variables",
   comps = c(1, 2), where = c("t", "t"), cex = 1,
   col.xlabels = "#5592e3", col.ylabels = "#fe9429",
   yfont = 2, pos = NULL, offset = 0.1,
   col.xarrows = "#5b9cf255", col.yarrows = "#fe942955",
   lwd = 3, length = 0, angle = 0, col.points = "#5592e3",
   pch = 21, pt.bg = "#5b9cf255", show.names = FALSE,
   xpd = TRUE, xlab = NULL, ylab = NULL, main = NULL,
   col.main = "gray35", cex.main = 1.2,
   col.axis = "gray40", show.grid = TRUE,
   col.grid = "gray95", ...)
```

#### **Arguments**

x An object of class "plsreg2".

what What to plot. Options are "variables" and "observations".

comps An integer vector of length two to indicate which components to plot.

where Where to plot the observations. A character vector of length two to indicate

which components to use when plotting observations. This parameter will take into account the values in comps. Possible options are: c("t", "u") for using x-y components, c("t", "t"), for using x components, and c("u", "u") for using

y components. Default c("t", "t").

cex Character expansion for labels and points.

col.xlabels Color for labels of X-block variables.
col.ylabels Color for labels of Y-block variables.

yfont Integer for specifying which font to use for Y-block labels. See font in graphical

parameters par.

pos Position for the text (see graphical paramaters par).

offset When pos is specified, this value gives the offset of the labels.

col.xarrows Color for the X-block arrows.

col.yarrows Color for the Y-block arrows.

lwd The line width of arrows.

length Length of the edges of the arrow head (in inches).

angle Angle from the shaft of the arrow to the edge of the arrow head.

col.points Color for the points when what="observations".

pch Plotting character symbol to use (see par).

pt.bg Background (fill) color for the points given by pch=21:25.

show.names Logical indicating whether to show labels of points. Only used when what="observations".

xpd Logical for controlling clipping region of names and labels.

xlab A title for the x axis.

ylab	A title for the y axis.
main	Main title of the plot.
col.main	Color of main title.
cex.main	Character expansion of main title.
col.axis	Color of axis annotations (tick marks and labels).
show.grid	Logical indicating whether to show grid lines.
col.grid	Color of grid lines. Only used when show.grid=TRUE.
	Further arguments are passed to labels or points.

#### **Details**

Variables are displayed using the correlations of each block of variables with its set of components: \$cor.xt and \$cor.yt.

## Author(s)

Gaston Sanchez

## See Also

```
plsreg2
```

```
## Not run:
    # load dataset vehicles
    data(vehicles)

# apply plsreg2
pls2 = plsreg2(vehicles[,1:12], vehicles[,13:16])

# plot variables (circle of correlations)
plot(pls2, what="variables")

# plot observations (as points)
plot(pls2, what="observations")

# plot observations with labels
plot(pls2, what="observations", show.names=TRUE)

## End(Not run)
```

20 plot.simpls

## **Description**

Plot method for objects of class "simpls". This function plots either the variables or the observations, on the selected components (i.e. scores). Variables are plotted inside the circle of correlations. Observations are plotted on a scatter plot.

## Usage

```
## S3 method for class 'simpls'
plot(x, what = "variables",
   comps = c(1, 2), cex = 1, col.xlabels = "#5592e3",
   col.ylabels = "#fe9429", yfont = 2, pos = NULL,
   offset = 0.1, col.xarrows = "#5b9cf255",
   col.yarrows = "#FE992955", lwd = 3, length = 0,
   angle = 0, col.points = "#5592e3", pch = 21,
   pt.bg = "#5b9cf255", show.names = FALSE, xpd = TRUE,
   xlab = NULL, ylab = NULL, main = NULL,
   col.main = "gray35", cex.main = 1.2,
   col.axis = "gray40", show.grid = TRUE,
   col.grid = "gray95", ...)
```

## **Arguments**

X	An object of class "simpls".
what	What to plot. Options are "variables" and "observations"
comps	An integer vector of length two to indicate which components to plot
cex	Character expansion for labels and points.
col.xlabels	Color for labels of X-block variables.
col.ylabels	Color for labels of Y-block variables.
yfont	Integer for specifying which font to use for Y-block labels. See font in graphical parameters par.
pos	Position for the text (see graphical paramaters par).
offset	When pos is specified, this value gives the offset of the label.
col.xarrows	Color for the X-block arrows.
col.yarrows	Color for the Y-block arrows.
lwd	The line width of arrows.
length	Length of the edges of the arrow head (in inches).
angle	Angle from the shaft of the arrow to the edge of the arrow head.
col.points	Color for the points when what="observations".

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pch Plotting character symbol to use (see par).pt.bg Background (fill) color for the points given by pch=21:25.

show.names Logical indicating whether to show labels of points. Only used when what="observations"

xpd Logical for controlling clipping region of names and labels.

xlab A title for the x axis.
ylab A title for the y axis.
main Main title of the plot.
col.main Color of main title.

cex.main Character expansion of main title.

col.axis Color of axis annotations (tick marks and labels). show.grid Logical indicating whether to show grid lines.

col.grid Color of grid lines. Only used when show.grid=TRUE.

... Further arguments are passed to labels or points.

#### **Details**

Variables are displayed using the correlations of each block of variables with the X-components: \$cor.xt and \$cor.yt.

## Author(s)

Gaston Sanchez

#### See Also

simpls

```
## Not run:
    # load dataset linnerud
    data(linnerud)

# apply simpls
    sim = simpls(linnerud[,1:3], linnerud[,4:6])

# plot variables (circle of correlations)
    plot(sim, what="variables")

# plot observations (as points)
    plot(sim, what="observations")

# plot observations with names
    plot(sim, what="observations", show.names=TRUE)

## End(Not run)
```

22 plot.simplsca

plot.simplsca

Plot SIMPLS-CA basic results

#### **Description**

Plot method for objects of class "simplsca". This function plots either the variables or the observations, on the selected components (i.e. scores). Variables are plotted inside the circle of correlations. Observations are plotted on a scatter plot.

## Usage

```
## S3 method for class 'simplsca'
plot(x, what = "variables",
   comps = c(1, 2), where = c("t", "t"), cex = 1,
   col.xlabels = "#5592e3", col.ylabels = "#fe9429",
   yfont = 2, pos = NULL, offset = 0.1,
   col.xarrows = "#5b9cf255", col.yarrows = "#fe942955",
   lwd = 3, length = 0, angle = 0, col.points = "#5592e3",
   pch = 21, pt.bg = "#5b9cf255", show.names = FALSE,
   xpd = TRUE, xlab = NULL, ylab = NULL, main = NULL,
   col.main = "gray35", cex.main = 1.2,
   col.axis = "gray40", show.grid = TRUE,
   col.grid = "gray95", ...)
```

## **Arguments**

X	An object of class "simplsca".
what	What to plot. Options are "variables" and "observations".
comps	An integer vector of length two to indicate which components to plot.
where	Where to plot the observations. A character vector of length two to indicate which components to use when plotting observations. This parameter will take into account the values in comps. Possible options are: $c("t","u")$ for using x-y components, $c("t","t")$ , for using x components, and $c("u","u")$ for using y components. Default $c("t","t")$ .
cex	Character expansion for labels and points.
col.xlabels	Color for labels of X-block variables.
col.ylabels	Color for labels of Y-block variables.
yfont	Integer for specifying which font to use for Y-block labels. See font in graphical parameters par.
pos	Position for the text (see graphical paramaters par)
offset	When pos is specified, this value gives the offset of the label
col.xarrows	Color for the X-block arrows.
col.yarrows	Color for the Y-block arrows.

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1wd The line width of arrows.

length Length of the edges of the arrow head (in inches).

angle Angle from the shaft of the arrow to the edge of the arrow head.

col.points Color for the points when what="observations".

pch Plotting character symbol to use (see par).

pt.bg Background (fill) color for the points given by pch=21:25.

show.names Logical indicating whether to show labels of points. Only used when what="observations".

xpd Logical for controlling clipping region of names and labels.

xlab A title for the x axis.
ylab A title for the y axis.
main Main title of the plot.
col.main Color of main title.

cex.main Character expansion of main title.

col.axis Color of axis annotations (tick marks and labels). show.grid Logical indicating whether to show grid lines.

col.grid Color of grid lines. Only used when show.grid=TRUE.

... Further arguments are passed to labels or points.

#### **Details**

Variables are displayed using the correlations of each block of variables with its set of components: \$cor.xt and \$cor.yu.

#### Author(s)

Gaston Sanchez

#### See Also

simplsca

```
## Not run:
# load dataset linnerud
data(linnerud)

# apply simplsca
simca = simplsca(linnerud[,1:3], linnerud[,4:6])

# plot variables (circle of correlations)
plot(simca, what="variables")

# plot observations (as points) using components (t1,u1)
plot(simca, what="observations", comps=c(1,1), where=c("t","u"))
```

24 plsca

plsca

PLS-CA: Partial Least Squares Canonical Analysis

## Description

Performs partial least squares canonical analysis for two blocks of data. Compared to PLSR2, the blocks of variables in PLS-CA play a symmetric role (i.e. there is neither predictors nor responses)

## Usage

```
plsca(X, Y, comps = NULL, scaled = TRUE)
```

#### **Arguments**

X	A numeric matrix or data frame (X-block) with more than one variable. No missing data are allowed
Υ	A numeric matrix or data frame (Y-block) with more than one variable. No missing data are allowed
comps	The number of extracted PLS components (NULL by default) When comps=NULL the number of components is determined by taking the minimum between the number of columns from X and Y.
scaled	A logical value indicating whether scaling data should be performed (TRUE by default). #'When scaled=TRUE the data is scaled to standardized values (mean=0, variance=1). Otherwise the data will only be centered (mean=0).

## Value

An object of class "plsca", basically a list with the following elements:

x.scores	scores of the X-block (also known as T components)
x.wgs	weights of the X-block
x.loads	loadings of the X-block
v.scores	scores of the Y-block (also known as U components)

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y.wgs	weights of the Y-block
y.loads	loadings of the Y-block
cor.xt	correlations between X and T
cor.yu	correlations between Y and U
cor.tu	correlations between T and U
cor.xu	correlations between X and U
cor.yt	correlations between Y and T
R2X	explained variance of X by T
R2Y	explained variance of Y by U
com.xu	communality of X with U
com.yt	communality of Y with T

## Author(s)

Gaston Sanchez

## References

Tenenhaus, M. (1998) La Regression PLS. Theorie et Pratique. Editions TECHNIP, Paris.

#### See Also

```
plot.plsca
```

```
## Not run:
## example of PLSCA with the vehicles dataset
data(vehicles)

# apply plsca
my_plsca = plsca(vehicles[,1:12], vehicles[,13:16])
my_plsca

# plot variables
plot(my_plsca)

## End(Not run)
```

26 plsreg1

plsreg1	PLS-R1: Partial Least Squares Regression 1	

## Description

The function plsreg1 performs Partial Least Squares Regression for the univariate case (i.e. one response variable)

#### **Usage**

```
plsreg1(predictors, response, comps = 2, crosval = TRUE)
```

## Arguments

predictors A numeric matrix or data frame with the predictor variables (which may contain

missing data).

response A numeric vector for the reponse variable. No missing data allowed.

comps The number of extracted PLS components (2 by default).

crosval Logical indicating whether cross-validation should be performed (TRUE by de-

fault). No cross-validation is done if there is missing data or if there are less

than 10 observations.

#### **Details**

The minimum number of PLS components (comps) to be extracted is 2.

The data is scaled to standardized values (mean=0, variance=1).

The argument crosval gives the option to perform cross-validation. This parameter takes into account how comps is specified. When comps=NULL, the number of components is obtained by cross-validation. When a number of components is specified, cross-validation results are calculated for each component.

#### Value

An object of class "plsreg1", basically a list with the following elements:

x.scores	PLS components (also known as T-components)
x.loads	loadings of the predictor variables
y.scores	scores of the response variable (also known as U-components)
y.loads	loadings of the response variable
cor.xyt	Correlations between the variables and the PLS components
raw.wgs	weights to calculate the PLS scores with the deflated matrices of predictor variables
mod.wgs	modified weights to calculate the PLS scores with the matrix of predictor variables

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std.coefs	Vector of standardized regression coefficients
reg.coefs	Vector of regression coefficients (used with the original data scale)
R2	Vector of PLS R-squared
R2Xy	explained variance of variables by PLS-components
y.pred	Vector of predicted values
resid	Vector of residuals
T2	Table of Hotelling T2 values (used to detect atypical observations)
Q2	Table with the cross validation results. Includes: PRESS, RSS, Q2, and cummulated Q2. Only available when crosval=TRUE

#### Author(s)

Gaston Sanchez

#### References

Geladi, P., and Kowalski, B. (1986) Partial Least Squares Regression: A Tutorial. *Analytica Chimica Acta*, **185**, pp. 1-17.

Tenenhaus, M. (1998) La Regression PLS. Theorie et Pratique. Editions TECHNIP, Paris.

Tenenhaus, M., Gauchi, J.-P., and Menardo, C. (1995) Regression PLS et applications. *Revue de statistique appliquee*, **43**, pp. 7-63.

## See Also

```
plot.plsreg1, plsreg2.
```

```
## Not run:
    ## example of PLSR1 with the vehicles dataset
    # predictand variable: price of vehicles
    data(vehicles)

# apply plsreg1 extracting 2 components (no cross-validation)
    pls1_one = plsreg1(vehicles[,1:12], vehicles[,13,drop=FALSE], comps=2, crosval=FALSE)

# apply plsreg1 with selection of components by cross-validation
    pls1_two = plsreg1(vehicles[,1:12], vehicles[,13,drop=FALSE], comps=NULL, crosval=TRUE)

# apply plsreg1 extracting 5 components with cross-validation
    pls1_three = plsreg1(vehicles[,1:12], vehicles[,13,drop=FALSE], comps=5, crosval=TRUE)

# plot variables
    plot(pls1_one)

## End(Not run)
```

28 plsreg2

plsreg2	PLS-R2: Partial Least Squares Regression 2	
---------	--	--

## **Description**

The function plsreg2 performs partial least squares regression for the multivariate case (i.e. more than one response variable)

## Usage

```
plsreg2(predictors, responses, comps = 2, crosval = TRUE)
```

#### **Arguments**

predictors A numeric matrix or data frame containing the predictor variables.

A numeric matrix or data frame containing the response variables.

The number of extracted PLS components (2 by default)

Crosval Logical indicating whether cross-validation should be performed (TRUE by default). No cross-validation is done if there is missing data or if there are less

than 10 observations.

#### **Details**

The minimum number of PLS components comps to be extracted is 2.

The data is scaled to standardized values (mean=0, variance=1).

The argument crosval gives the option to perform cross-validation. This parameter takes into account how comps is specified. When comps=NULL, the number of components is obtained by cross-validation. When a number of components is specified, cross-validation results are calculated for each component.

#### Value

An object of class "plsreg2", basically a list with the following elements:

x.scores	components of the predictor variables (also known as T-components)
x.loads	loadings of the predictor variables
y.scores	components of the response variables (also known as U-components)
y.loads	loadings of the response variables
cor.xt	correlations between X and T
cor.yt	correlations between Y and T
cor.xu	correlations between X and U
cor.yu	correlations between Y and U
cor.tu	correlations between T and U

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raw.wgs	weights to calculate the PLS scores with the deflated matrices of predictor variables
mod.wgs	modified weights to calculate the PLS scores with the matrix of predictor variables
std.coefs	Vector of standardized regression coefficients (used with scaled data)
reg.coefs	Vector of regression coefficients (used with the original data)
y.pred	Vector of predicted values
resid	Vector of residuals
expvar	table with R-squared coefficients
VIP	Variable Importance for Projection
Q2	table of Q2 indexes (i.e. leave-one-out cross validation)
Q2cum	table of cummulated Q2 indexes

#### Author(s)

Gaston Sanchez

#### References

Geladi, P., and Kowlaski, B. (1986) Partial Least Squares Regression: A Tutorial. *Analytica Chimica Acta*, **185**, pp. 1-17.

Hoskuldsson, A. (1988) PLS Regression Methods. Journal of Chemometrics, 2, pp. 211-228.

Tenenhaus, M. (1998) La Regression PLS. Theorie et Pratique. Editions TECHNIP, Paris.

#### See Also

```
plot.plsreg2, plsreg1.
```

```
## Not run:
## example of PLSR2 with the vehicles dataset
data(vehicles)

# apply plsreg2 extracting 2 components (no cross-validation)
pls2_one = plsreg2(vehicles[,1:12], vehicles[,13:16], comps=2, crosval=FALSE)

# apply plsreg2 with selection of components by cross-validation
pls2_two = plsreg2(vehicles[,1:12], vehicles[,13:16], comps=NULL, crosval=TRUE)

# apply plsreg2 extracting 5 components with cross-validation
pls2_three = plsreg2(vehicles[,1:12], vehicles[,13:16], comps=5, crosval=TRUE)

# plot variables
plot(pls2_one)

## End(Not run)
```

30 simpls

ropes	Climbing Ropes data set
	G I

## Description

This dataset gives the measurements of 101 climbing ropes available in the market by spring 2011. The data was collected from the brands websites.

## Usage

```
data(ropes)
```

#### **Format**

A data frame with 101 observations on the following 7 variables.

Num	Variable	Description
1	brand	a factor with the brand names
2	diameter	the diameter of the ropes measured in mm
3	weight	the weight measured in grams per meter
4	falls	the number of UIAA falls
5	imp.force	the impact force value
6	stat.elong	the static elongation value
7	dyn.elong	the dynamic elongation value

## Source

Personal collection of data. (Gaston Sanchez)

## **Examples**

```
data(ropes)
summary(ropes)
```

simpls

SIMPLS: Alternative Approach to PLS Regression

## **Description**

The function simpls performs the SIMPLS Algorithm as described in Michel Tenenhaus book *La Regression PLS*, chapter 5.

## Usage

```
simpls(X, Y, comps = 2)
```

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## **Arguments**

Χ	Numeric matrix or data frame with two or more columns (X-block).
Υ	Numeric matrix or data frame with two or more columns (Y-block).

comps Number of components to be extracted. (TRUE by default).

#### **Details**

No missing data are allowed.

#### Value

An object of class "simpls", basically a list with the following elements:

x.scores	scores of the X-block (also known as T components)
x.wgs	weights of the X-block
y.wgs	weights of the Y-block
cor.xt	correlations between X and T
cor.yt	correlations between Y and T
R2X	explained variance of X by T
R2Y	explained variance of Y by T

## Author(s)

Gaston Sanchez

## References

Tenenhaus, M. (1998) *La Regression PLS. Theorie et Pratique*. Paris: Editions TECHNIP. de Jong, S. (1993) SIMPLS: An alternative approach to partial least squares regression. *Chemometrics and Intelligent Laboratory Systems*, 18: 251-263.

#### See Also

```
plot.simpls, simplsca
```

```
## Not run:
# load data linnerud
data(linnerud)

# apply inter-battery method
my_simpls = simpls(linnerud[,1:3], linnerud[,4:6])

# plot variables
plot(my_simpls, what="variables")

## End(Not run)
```

32 simplsca

simplsca

SIMPLS-CA: SIMPLS Canonical Analysis

## Description

The function simplsca performs the SIMPLS Canonical Analysis algorithm as described in Michel Tenenhaus book *La Regression PLS*, chapter 5.

## Usage

```
simplsca(X, Y, comps = 2)
```

## Arguments

Χ	Numeric matrix or data frame with two or more columns (X-block).
Υ	Numeric matrix or data frame with two or more columns (Y-block).
comps	Number of components to be extracted. (TRUE by default).

## **Details**

No missing data are allowed.

#### Value

An object of class "simplsca", basically a list with the following elements:

x.scores	scores of the X-block (also known as T components)
x.wgs	weights of the X-block
y.scores	scores of the Y-block (also known as U components)
y.wgs	weights of the Y-block
cor.xt	correlations between X and T
cor.yu	correlations between Y and U
cor.xu	correlations between X and U
cor.yt	correlations between Y and T
cor.tu	correlations between T and U
R2XT	explained variance of X by T
R2YT	explained variance of Y by T
R2YU	explained variance of Y by U
R2XU	explained variance of X by U

## Author(s)

Gaston Sanchez

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#### References

Tenenhaus, M. (1998) La Regression PLS. Theorie et Pratique. Paris: Editions TECHNIP.

#### See Also

```
plot.simplsca, simpls
```

## **Examples**

```
## Not run:
# load data linnerud
data(linnerud)

# apply inter-battery method
my_simca = simplsca(linnerud[,1:3], linnerud[,4:6])

# plot variables
plot(my_simca, what="variables")

## End(Not run)
```

vehicles

Vehicles data set

## Description

These data are the specification of 30 vehicles in terms of various characteristics.

#### **Format**

A data frame with 30 observations and 16 variables.

Num	Variable	Description
1	diesel	Diesel fuel-type
2	turbo	Turbo aspiration
3	two.doors	Vechicles with two doors
4	hatchback	Hatchback body-style
5	wheel.base	Wheel base
6	length	Length
7	width	Width
8	height	Height
9	curb.weight	Curb weight
10	eng.size	Engine size
11	horsepower	Horsepower
12	peak.rpm	Peak revolutions per minute
13	price	Price in dollars
14	symbol	Insurance risk rating
15	city.mpg	Fuel consume in city

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## 16 highway.mpg Fuel consume in highway

## Source

- 1) 1985 Model Import Car and Truck Specifications, 1985 Ward's Automotive Yearbook.
- 2) Personal Auto Manuals, Insurance Services Office, 160 Water Street, New York, NY 10038.
- 3) Insurance Collision Report, Insurance Institute for Highway Safety, Watergate 600, Washington, DC 20037.

Machine Learning Repository. https://archive.ics.uci.edu/ml/datasets/Automobile

## **Examples**

data(vehicles)
vehicles

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