# Package 'morepls'

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Title Interpretation Tools for Partial Least Squares Regression

Type Package

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| <b>Description</b> Various kinds of plots (observations, variables, correlations, weights, regression coefficients and Variable Importance in the Projection) and aids to interpretation (coefficients, Q2, correlations, redundancies) for partial least squares regressions computed with the 'pls' package, following Tenenhaus (1998, ISBN:2-7108-0735-1). |
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get\_coef

Standardized and raw coefficients

### **Description**

Computes the standardized and raw coefficients of a PLS regression, with p-values and confidence intervals from a jackknife procedure.

### Usage

```
get_coef(object, y = NULL, ncomp = NULL,
  ci = 0.95, raw = FALSE)
```

### **Arguments**

| object | an object of class mvr from pls package. It must be cross-validated with jackknife = TRUE                                 |
|--------|---|
| У      | the name of the response variable whose coefficients are plotted. If NULL (default), the first response variable is used. |
| ncomp  | the number of components to use for computing coefficients  |
| ci     | the confidence level of the confidence interval. Default is 0.95.   |
| raw    | logical. If FALSE (default), standardized coefficients are computed. If TRUE, raw coefficients are computed.              |

#### Value

A data frame with coefficients, standard deviation, t-values, p-values and confidence intervals.

### Author(s)

Nicolas Robette

#### References

```
Martens, H., Næs, T. (1989) Multivariate calibration. Chichester: Wiley.
Tenenhaus, M. (1998) La Regression PLS. Theorie et Pratique. Editions TECHNIP, Paris.
```

### See Also

```
plo_coef
```

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#### **Examples**

get\_cor

Correlations between variables and scores

### **Description**

Computes correlations between variables and scores from a PLS regression.

### Usage

```
get_cor(object)
```

### Arguments

object an object of class mvr from pls package.

#### Value

A list with the following elements:

| Xt | correlations between X variables and X scores    |
|----|--|
| Yt | correlations between Y variables and X scores    |
| Xu | correlations between X variables and Y scores    |
| Yu | correlations between Y variables and Y scores    |
| XY | correlations between X variables and Y variables |
| tu | correlations between X scores and Y scores       |

### Author(s)

Nicolas Robette

#### References

```
Martens, H., Næs, T. (1989) Multivariate calibration. Chichester: Wiley.
```

get\_Q2

#### See Also

```
get_red, plo_cor
```

#### **Examples**

get\_Q2

Q2 and cumulative Q2 indexes

### Description

Computes Q2 and cumulative Q2 indexes from a PLS regression.

#### Usage

```
get_Q2(object)
```

### **Arguments**

object an object of class mvr from pls package. It has to be cross-validated

#### Value

A list with the following elements:

Q2kh Q2 index by X variable and number of components

Q2 index by number of components

Q2cumkh cumulative Q2 index by X variable and number of components

Q2cumh cumulative Q2 index by number of components

#### Author(s)

Nicolas Robette

#### References

Martens, H., Næs, T. (1989) Multivariate calibration. Chichester: Wiley.

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#### **Examples**

get\_red

R2 and redundancies

### Description

Computes R2 and redundancies between variables and scores from a PLS regression.

#### Usage

```
get_red(object)
```

#### **Arguments**

object

an object of class mvr from pls package.

#### Value

A list with the following elements:

| Xt    | R2 and redundancies between X variables and X scores   |
|-------|--|
| Yt    | R2 and redundancies between Y variables and X scores   |
| Xu    | R2 and redundancies between X variables and Y scores   |
| Yu    | R2 and redundancies between Y variables and Y scores   |
| Xtcum | cumulative R2 and redundancies between X variables and |

Xtcum cumulative R2 and redundancies between X variables and X scores cumulative R2 and redundancies between Y variables and X scores Xucum cumulative R2 and redundancies between X variables and Y scores Yucum cumulative R2 and redundancies between Y variables and Y scores

#### Author(s)

Nicolas Robette

### References

```
Martens, H., Næs, T. (1989) Multivariate calibration. Chichester: Wiley.
```

plo\_coef

### See Also

```
get_cor
```

### **Examples**

plo\_coef

Plot of coefficients

## Description

Plots the coefficients from a PLS regression.

### Usage

### Arguments

| object   | an object of class mvr from pls package   |
|----------|---|
| У        | the name of the response variable whose coefficients are plotted. If NULL (default), the first response variable is used.   |
| ncomp    | the number of components to use for computing coefficients  |
| sort     | logical. If TRUE, bars are sorted by decreasing coefficients. Default is FALSE.   |
| col      | color of the bars   |
| repel    | logical. If TRUE, the names of the variables are repelled with <code>geom_text_repel</code> . Default is <code>FALSE</code>   |
| max.pval | coefficients with jack-knife p-values higher than max.pval have a more transparent color bar. If NULL (default), all bars have the same opacity. If not NULL, object must be cross-validated with jackknife = TRUE. |
| whiskers | logical. If TRUE, whiskers are added to represent the confidence interval of the coefficients. Default is FALSE. If TRUE, object must be cross-validated with jackknife = TRUE.                                     |
| ci       | the confidence level of the confidence interval. Only used if whiskers is TRUE. Default is 0.95.  |

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### Value

```
a ggplot2 object
```

#### Author(s)

Nicolas Robette

#### References

```
Martens, H., Næs, T. (1989) Multivariate calibration. Chichester: Wiley. Tenenhaus, M. (1998) La Regression PLS. Theorie et Pratique. Editions TECHNIP, Paris.
```

### See Also

```
plo_ctr, plo_vip, jack.test,
```

### **Examples**

plo\_cor

Plot of correlations

### **Description**

Plots the correlations between (X and Y) variables and the components (X scores) of a PLS regression.

#### Usage

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### **Arguments**

| object  | an object of class mvr from pls package   |
|---------|---|
| comps   | the components to use. Default is $c(1,2)$ .  |
| which   | character string. If "both" (default), X and Y variables are plotted. If "X", only X variables are plotted. If "Y", only Y variables are plotted.                                     |
| min.cor | numerical value. The minimal correlation with one or the other component for a variable to be plotted. If NULL (default), all the variables are plotted.                              |
| lim     | numerical value. The limit of the scale (in absolute value). If NULL (default), the limits are automatically determined from the range of tha data.                                   |
| circles | vector of numeric values. Circles are added to the plot at radiuses specified in circles. If NULL (default), no circle is plotted.  |
| col     | colors for the names of the variables. Only one value should be provided if which is "X" or "Y", a vector of two if which is "both". If NULL (default), colors are set automatically. |
| size    | numerical value. The size of the names of the variables.  |

### Value

```
a ggplot2 object
```

#### Note

This is what Tenenhaus calls the univariate interpretation of the PLS components, as opposed to the multivariate interpretation (see plo\_var).

### Author(s)

Nicolas Robette

### References

```
Martens, H., Næs, T. (1989) Multivariate calibration. Chichester: Wiley.
Tenenhaus, M. (1998) La Regression PLS. Theorie et Pratique. Editions TECHNIP, Paris.
```

### See Also

```
get_cor, plo_var
```

## Examples

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```
plo_cor(pls)
# plot with circles corresponding to
# correlations of 0.5 and 1
plo_cor(pls, lim = 1, circles = c(0.5, 1), col = c("pink", "purple"))
```

plo\_ctr

Plot of weights

### **Description**

Plots the weights of X variables from a PLS regression.

### Usage

```
plo_ctr(object, comp = 1, sort = FALSE, col = "tomato4", repel = FALSE)
```

#### **Arguments**

| object | an object of class mvr from pls package  |
|--------|--|
| comp   | the component to use. Default is 1.  |
| sort   | logical. If TRUE, bars are sorted by decreasing VIPs. Default is FALSE.                          |
| col    | color of the bars  |
| repel  | logical. If TRUE, the names of the variables are repelled with geom_text_repel. Default is FALSE |

According to Tenenhaus, the contribution of a variable to the construction of a component is measured by the squared loading weight. For a given component, the sum af the squared loading weights is equal to 1. This plot represents the loading weights, which keeps the information about their sign. Dashed lines are added at +/- sqrt(1/p), with p the number of X variables, which corresponds to the average contribution to the construction of the component.

#### Value

**Details** 

```
a ggplot2 object
```

#### Author(s)

Nicolas Robette

#### References

```
Martens, H., Næs, T. (1989) Multivariate calibration. Chichester: Wiley.
```

plo\_inter

### See Also

```
plo_coef, plo_vip
```

### **Examples**

plo\_inter

Plot of Interactions

## Description

Plots the interaction between two categorical supplementary variables for a PLS regression.

### Usage

```
plo_inter(object, var1, var2, excl1 = NULL, excl2 = NULL,
  comps = c(1,2), shapesize = 1, textsize = 3,
  force = 1, max.overlaps = Inf,
  lines = TRUE, dashes = TRUE)
```

### **Arguments**

| object       | an object of class mvr from pls package   |
|--------------|---|
| var1         | factor. The first categorical supplementary variable.   |
| var2         | factor. The second categorical supplementary variable.  |
| excl1        | character vector of categories from the var1 to exclude from the plot. If NULL (default), all the supplementary categories are plotted. |
| excl2        | character vector of categories from the var2 to exclude from the plot. If NULL (default), all the supplementary categories are plotted. |
| comps        | the components to use. Default is $c(1,2)$ .  |
| shapesize    | Size of the shapes. Default is 1.   |
| textsize     | Size of the labels of categories. Default is 3.   |
| force        | Force of repulsion between overlapping text labels. Defaults to 1. If 0, labels are not repelled at all.                                |
| max.overlaps | Exclude text labels that overlap too many things. Defaults to Inf, which means no labels are excluded.                                  |

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lines logical. Whether to add colored lines between the points of the categories of v1.

Default is TRUE.

dashes logical. Whether to add gray dashed lines between the points of the categories

of v2. Default is TRUE.

#### Value

```
a ggplot2 object
```

#### Author(s)

Nicolas Robette

#### References

```
Martens, H., Næs, T. (1989) Multivariate calibration. Chichester: Wiley.
```

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

#### See Also

```
plo_sup, plo_part
```

### **Examples**

plo\_obs

Plot of scores

#### **Description**

Plots the scores of the observations of a PLS regression.

### Usage

```
plo_obs(object, comps = 1:2, col = "black", size = 1.5)
```

plo\_part

### Arguments

```
object an object of class mvr from pls package comps the components to use. Default is c(1,2). col the color of the points.

size numerical value. The size of the points.
```

#### Value

```
a ggplot2 object
```

### Author(s)

Nicolas Robette

#### References

```
Martens, H., Næs, T. (1989) Multivariate calibration. Chichester: Wiley.
Tenenhaus, M. (1998) La Regression PLS. Theorie et Pratique. Editions TECHNIP, Paris.
```

### **Examples**

plo\_part

Plot of Main and Partial Effect

### Description

Plots the the main and partial effects of a supplementary variable for a PLS regression, with one or more supplementary partialled out.

### Usage

```
plo_part(object, var, controls, excl = NULL,
  comps = c(1,2), shapesize = 1.5, col = "black",
  textsize = 4, force = 1, max.overlaps = Inf,
  lines = TRUE, dashes = TRUE, alpha = 0.3, legend = "right")
```

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#### Arguments

object an object of class mvr from pls package

var factor. The categorical supplementary variable.

controls data frame of supplementary variables to be partialled out (i.e. control variables)

excl character vector of categories from the var to exclude from the plot. If NULL

(default), all the supplementary categories are plotted.

comps the components to use. Default is c(1,2).

shapesize Size of the shapes. Default is 1.5.

col the color for the labels and lines. Default is "black".

textsize Size of the labels of categories. Default is 4.

force Force of repulsion between overlapping text labels. Defaults to 1. If 0, labels

are not repelled at all.

max.overlaps Exclude text labels that overlap too many things. Defaults to Inf, which means

no labels are excluded.

lines logical. Whether to add colored lines between the points of the categories of v1.

Default is TRUE.

dashes logical. Whether to add gray dashed lines between the points of the categories

of v2. Default is TRUE.

alpha Numerical value. Transparency of the partial effects. Default is 0.3.

legend the position of legends ("none", "left", "right", "bottom", "top", or two-element

numeric vector). Default is right.

#### Value

a ggplot2 object

#### Note

The partial effects of the supplementary variable are computed with the Average Marginal Effects of a linear regression, with individual coordinates as dependent variable, and the supplementary and control variables as independent variables.

#### Author(s)

Nicolas Robette

#### References

Martens, H., Næs, T. (1989) Multivariate calibration. Chichester: Wiley.

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

#### See Also

plo\_sup, plo\_inter

plo\_sup

### **Examples**

plo\_sup

Plot of Supplementary Variables

### Description

Plots the categories of supplementary variables for a PLS regression.

### Usage

```
plo_sup(object, vars, excl = NULL, comps = c(1,2),
    shapesize = 2, textsize = 3, vlab = TRUE, force = 1,
    max.overlaps = Inf, dashes = TRUE)
```

### **Arguments**

| object       | an object of class mvr from pls package  |
|--------------|--|
| vars         | A data frame of categorical supplementary variables. All these variables should be factors.  |
| excl         | character vector of supplementary categories to exclude from the plot, specified in the form "namevariable.namecategory" (for instance "Gender.Men"). If NULL (default), all the supplementary categories are plotted. |
| comps        | the components to use. Default is $c(1,2)$ .   |
| shapesize    | Size of the shapes. Default is 2.  |
| textsize     | Size of the labels of categories. Default is 3.  |
| vlab         | Logical. If TRUE (default), the variable name is added as a prefix for the labels of the categories.   |
| force        | Force of repulsion between overlapping text labels. Defaults to 1. If 0, labels are not repelled at all.   |
| max.overlaps | Exclude text labels that overlap too many things. Defaults to Inf, which means no labels are excluded.   |
| dashes       | Logical. Should one add lines between categories? Default is TRUE.   |

### Value

```
a ggplot2 object
```

plo\_var

#### Author(s)

Nicolas Robette

#### References

```
Martens, H., Næs, T. (1989) Multivariate calibration. Chichester: Wiley.
Tenenhaus, M. (1998) La Regression PLS. Theorie et Pratique. Editions TECHNIP, Paris.
```

#### See Also

```
plo_var
```

### **Examples**

plo\_var

Plot of loadings

### **Description**

Plots the loadings of the variables of a PLS regression.

### Usage

```
plo_var(object, comps = 1:2, which = "both", col = NULL,
    size = 3.88, Yline = TRUE, col.Yline = "firebrick3")
```

### Arguments

| object | an object of class mvr from pls package   |
|--------|---|
| comps  | the components to use. Default is c(1,2).   |
| which  | character string. If "both" (default), $X$ and $Y$ variables are plotted. If "X", only $X$ variables are plotted. If "Y", only $Y$ variables are plotted.                               |
| col    | colors for the names of the variables. Only one value should be provided if which is "X" or "Y", a vector of two if which is "both". If $NULL$ (default), colors are set automatically. |
| size   | numerical value. The size of the names of the variables   |

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Yline logical. If TRUE (default), a line is drawn through the origin and the coordinates

of the response variable, and a second line orthogonal to the first one. This is

aimed at facilitating the interpretation.

col. Yline the color of the lines drawn if Yline is TRUE. Default is "firebrick3".

#### Value

```
a ggplot2 object
```

#### Note

This is what Tenenhaus calls the multivariate interpretation of the PLS components, as opposed to the univariate interpretation provided by the correlations (see plo\_cor). This superposes Y loadings (vectors from the C matrix) and projections, i.e. modified weights (vectors of the W\* matrix).

### Author(s)

Nicolas Robette

#### References

```
Martens, H., Næs, T. (1989) Multivariate calibration. Chichester: Wiley.
```

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

### See Also

```
plo_cor
```

### **Examples**

plo\_vip

Plot of VIPs

### Description

Plots the Variable Importance in Projections (VIP) indexes of a PLS regression.

plo\_vip

### Usage

```
plo_vip(object, ncomp = NULL, sort = FALSE,
col = "steelblue4", repel = FALSE)
```

### Arguments

object an object of class mvr from pls package

ncomp the number of components to use for computing VIPs

sort logical. If TRUE, bars are sorted by decreasing VIPs. Default is FALSE.

col color of the bars

repel logical. If TRUE, the names of the variables are repelled with geom\_text\_repel.

Default is FALSE

#### Value

```
a ggplot2 object
```

### Author(s)

Nicolas Robette

### References

```
Martens, H., Næs, T. (1989) Multivariate calibration. Chichester: Wiley.
Tenenhaus, M. (1998) La Regression PLS. Theorie et Pratique. Editions TECHNIP, Paris.
```

### See Also

VIP

### **Examples**

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