

Package ‘morepls’

March 9, 2024

Type Package

Title Interpretation Tools for Partial Least Squares Regression

Version 0.1

Imports pls, ggplot2, ggrepel, rlang

Suggests plsVarSel, ggforce

Description 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).

License GPL (>= 2)

Encoding UTF-8

RoxygenNote 7.2.3

NeedsCompilation no

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Repository CRAN

Date/Publication 2024-03-09 13:30:02 UTC

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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

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

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

See Also

[plo_coef](#)

Examples

```
library(pls)
data(yarn)
pls <- mvr(density ~ NIR,
           ncomp = 5,
           data = yarn,
           validation = "CV",
           method = "oscorespls",
           jackknife = TRUE)
res <- get_coef(pls)
head(res)
```

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

See Also

[get_red](#), [plo_cor](#)

Examples

```
library(pls)
data(yarn)
pls <- mvr(density ~ NIR,
           ncomp = 5,
           data = yarn,
           validation = "CV",
           method = "oscorespls")
res <- get_cor(pls)
str(res)
```

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
Q2h	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.
 Tenenhaus, M. (1998) La Regression PLS. Theorie et Pratique. Editions TECHNIP, Paris.

Examples

```
library(pls)
data(yarn)
pls <- mvr(density ~ NIR,
           ncomp = 5,
           data = yarn,
           validation = "CV",
           method = "oscorespls")
res <- get_Q2(pls)
str(res)
```

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

See Also[get_cor](#)**Examples**

```
library(pls)
data(yarn)
pls <- mvr(density ~ NIR,
           ncomp = 5,
           data = yarn,
           validation = "CV",
           method = "oscorespls")
res <- get_red(pls)
str(res)
```

`plo_coef`*Plot of coefficients*

Description

Plots the coefficients from a PLS regression.

Usage

```
plo_coef(object, y = NULL, ncomp = NULL, sort = FALSE,
         col = "darkgreen", repel = FALSE,
         max.pval = NULL, whiskers = FALSE, ci = 0.95)
```

Arguments

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

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

```
library(pls)
data(yarn)
pls <- mvr(density ~ NIR,
          ncomp = 5,
          data = yarn,
          validation = "CV",
          method = "oscorespls",
          jackknife = TRUE)
plo_coef(pls)
plo_coef(pls, max.pval = 0.05)
plo_coef(pls, whiskers = TRUE)
```

plo_cor

Plot of correlations

Description

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

Usage

```
plo_cor(object, comps = 1:2, which = "both", min.cor = NULL,
        lim = NULL, circles = NULL, col = NULL, size = 3.88)
```

Arguments

object	an object of class <code>mvr</code> from <code>pls</code> package
comps	the components to use. Default is <code>c(1, 2)</code> .
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 the 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

```
library(pls)
data(yarn)
pls <- mvr(density ~ NIR,
          ncomp = 5,
          data = yarn,
          validation = "CV",
          method = "oscorespls")
```



```
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 <code>mvr</code> from <code>pls</code> 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 <code>geom_text_repel</code> . Default is FALSE

Details

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 of 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 $\pm \sqrt{1/p}$, with p the number of X variables, which corresponds to the average contribution to the construction of the component.

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_coef](#), [plo_vip](#)

Examples

```
library(pls)
data(yarn)
pls <- mvr(density ~ NIR,
           ncomp = 5,
           data = yarn,
           validation = "CV",
           method = "oscorespls")
plo_ctr(pls)
```

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)
```

Arguments

object	an object of class <code>mvr</code> from <code>pls</code> package
comps	the components to use. Default is <code>c(1, 2)</code> .
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

```
library(pls)
data(yarn)
pls <- mvr(density ~ NIR,
           ncomp = 5,
           data = yarn,
           validation = "CV",
           method = "oscorespls")
plo_obs(pls)
```

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.
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

```
library(pls)
data(yarn)
pls <- mvr(density ~ NIR,
          ncomp = 5,
          data = yarn,
          validation = "CV",
          method = "oscorespls")
plo_var(pls)
```

plo_vip

Plot of VIPs

Description

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

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.

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

See Also

[VIP](#)

Examples

```
library(pls)
data(yarn)
pls <- mvr(density ~ NIR,
          ncomp = 5,
          data = yarn,
          validation = "CV",
          method = "oscorespls")
plo_vip(pls)
```

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