## Package 'Ispls'

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lspls-package LS-PLS Models

## Description

Implements the LS-PLS (least squares - partial least squares) method described in for instance Jørgensen, K., Segtnan, V. H., Thyholt, K., Næs, T. (2004) "A Comparison of Methods for Analysing Regression Models with Both Spectral and Designed Variables" Journal of Chemometrics, 18(10), 451-464, [doi:10.1002/cem.890](doi:10.1002/cem.890).

## Details

The DESCRIPTION file:

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| :--- | :--- |
| Title: | LS-PLS Models |
| Version: | $0.2-2$ |
| Date: | $2018-07-26$ |
| Authors@R: | c(person("Bjørn-Helge", "Mevik", role = c("aut", "cre"), email = "b-h@mevik.net")) |
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| Encoding: | UTF-8 |
| Depends: | pls (>= 2.2.0) |
| Imports: | grDevices, graphics, methods, stats |
| Description: | Implements the LS-PLS (least squares - partial least squares) method described in for instance Jørgensen, K., |
| License: | GPL-2 |
| URL: | http://mevik.net/work/software/lspls.html, https://github.com/bhmevik/lspls |
| BugReports: | https://github.com/bhmevik/lspls/issues |

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plot.lspls Plots of LS-PLS Models
plot.lsplsCv Plot Method for Cross-Validations
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project Projection and Orthogonalisation
```

LS-PLS (least squares-partial least squares) models are written on the form

$$
Y=X \beta+T_{1} \gamma_{1}+\cdots+T_{k} \gamma_{k}+E
$$

where the terms $T_{i}$ are one or more matrices $Z_{i, j}$ separated by a colon (:), i.e., $Z_{i, 1}: Z_{i, 2}: \cdots: Z_{i, l_{i}}$. Multi-response models are possible, in wich case $Y$ should be a matrix.
The model is fitted from left to right. First $Y$ is fitted to $X$ using least squares (LS) regression and the residuals calculated. For each $i$, the matrices $Z_{i, 1}, \ldots, Z_{i, l_{i}}$ are orthogonalised against the variables used in the regression sofar (when $i=1$, this means $X$ ). The residuals from the LS regression are used as the response in PLS regressions with the orthogonalised matrices as predictors (one PLS regression for each matrix), and the desired number of PLS components from each matrix are included among the LS prediction variables. The LS regression is then refit with the new variables, and new residuals calculated.
The function to fit LS-PLS models is lspls. A typical usage to fit the model

$$
y=X \beta+Z \gamma+V_{1}: V_{2} \eta+W \theta+E
$$

would be

```
mod <- lspls(y ~ X + Z + V1:V2 + W, ncomp = list(3, c(2,1), 2),
    data = mydata)
```

The first argument is the formula describing the model. X is fit first, using LS. Then PLS scores from Z (orthogonalised) are added. Then PLS scores from V1 and V2 are added (simultaneously), and finally PLS scores from W. The next argument, ncomp, specifies the number of components to use from each PLS: 3 Z score vectors, 2 V 1 score vectors, 1 V 2 score vector and 2 W score vectors. Finally, mydata should be a data frame with matrices $y, X, Z, V 1, V 2$ and $W$ (for single-response models, y can be a vector).
Currently, score plots and loading plots of fitted models are implemented. plot(mod, "scores") gives score plots for each PLS regression, and plot (mod, "loadings") gives loading plots.
There is a predict method to predict response or score values from new data

```
predict(mod, newdata = mynewdata)
```

(This predicts response values. Use type = "scores" to get scores.) Also, the standard functions resid and fitted can be used to extract the residuals and fitted values.

In order to determine the number of components to use from each matrix, one can use crossvalidation:

```
cvmod <- lsplsCv(y ~ X + Z + V1:V2 + W, ncomp = list(4, c(3,4), 3),
    segments = 12, data = mydata)
```

In lsplsCv, ncomp gives the maximal number of components to test. The argument segments specifies the number of segments to use. One can specify the type of segments to use (random (default), consequtive or interleaved) with the argument segment.type. Alternatively, one can supply the segments explicitly with segments. See lsplsCv for details.

One can plot cross-validated RMSEP values with plot (cvmod). (Similarly, plot (cvmod, "MSEP") plots MSEP values.) This makes it easier to determine the optimal number of components for each PLS. See plot. lsplsCv for details. To calculate the RMSEP or MSEP values explicitly, one can use the function RMSEP or MSEP.

## Author(s)

Bjørn-Helge Mevik [aut, cre]
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## References

Jørgensen, K., Segtnan, V. H., Thyholt, K., Næs, T. (2004) A Comparison of Methods for Analysing Regression Models with Both Spectral and Designed Variables. Journal of Chemometrics, 18(10), 451-464.
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## See Also

lspls, lsplsCV, plot.lspls, plot.lsplsCV

## Examples

\#\# FIXME

```
lspls
```

Fit LS-PLS Models

## Description

A function to fit LS-PLS (least squares-partial least squares) models.

## Usage

lspls(formula, ncomp, data, subset, na.action, model = TRUE, ...)

## Arguments

| formula | model formula. See Details. |
| :--- | :--- |
| ncomp | list or vector of positive integers, giving the number of components to use for <br> each 'pls-matrix'. See Details. <br> an optional data frame with the data to fit the model from. |
| data | an optional vector specifying a subset of observations to be used in the fitting <br> process. |
| subset | a function which indicates what should happen when the data contain missing <br> values. |
| model | logical. If TRUE, the model frame is returned. <br> additional arguments, passed to the underlying PLSR fit function. |
| $\ldots$ |  |

## Details

lspls fits LS-PLS models, in which matrices are added successively to the model. The first matrix is fit with ordinary least squares (LS) regression. The rest of the matrices are fit with partial least squares regression (PLSR), using the residuals from the preceeding model as response. See lsplspackage or the references for more details, and lspls-package for typical usage.

The model formula is specified as resp $\sim$ term1 + term $2+\ldots$. If resp is a matrix (with more than one coloumn), a multi-response model is fitted. term1 specifies the first matrix to be fitted, using LS. Each of the remaining terms will be added sequentially in the order specified in the formula (from left to right). Each term can either be a single matrix, which will be added by itself, or several matrices separated with :, e.g., Z:V:W, which will be added simultaneously (these will be denoted parallell matrices).
The first matrix, term1, is called the $L S$ matrix, and the rest of the predictor matrices (whether parallell or not) are called PLS matrices.

Note that an intercept is not automatically added to the model. It should be included as a constant coloumn in the LS matrix, if desired. (If no intercept is included, the PLS matrices should be centered. This happens automatically if the LS matrix includes the intercept.)

The number of components to use in each of the PLSR models is specified with the ncomp argument, which should be a list. Each element of the list gives the number of components to use for the corresponding term in the formula. If the term specifies parallell matrices (separated with :), the list element should be a vector with one integer for each matrix. Otherwise, it should be a number.
To simplify the specification of ncomp, the following conversions are made: if ncomp is a vector, it will be converted to a list. ncomp will also be recycled as neccessary to get one element for each term. Finally, for a parallell term, the list element will be recycled as needed. Thus, ncomp $=4$ will result in 4 components being fit for every PLS matrix.

Currently, the function lspls itself handles the formula and the data, and calls the underlying fit function orthlspls.fit to do the actual fitting. This implements the orthogonalized version of the LS-PLS algorithm, and without splitting of parallell matrices into common and unique components (see the references). Extensions to non-orthogonalized algorithms, and splitting of parallell matrices are planned.

## Value

An object of class "lspls". The object contains all components returned by the underlying fit function (currently orthlspls.fit). In addition, it contains the following components:
fitted.values matrix with fitted values, one coloumn per response
na.action if observations with missing values were removed, na. action contains a vector with their indices.
ncomp the list of number of components used in the model.
call the function call.
terms the model terms.
model if model = TRUE, the model frame.

## Note

The user interface (e.g. the model handling) is experimental, and might well change in later versions.

The handling of formula (especially :) is non-standard. Note that the order of the terms is significant; terms are added from left to right.

## Author(s)

Bjørn-Helge Mevik

## References

Jørgensen, K., Segtnan, V. H., Thyholt, K., Næs, T. (2004) A Comparison of Methods for Analysing Regression Models with Both Spectral and Designed Variables. Journal of Chemometrics, 18(10), 451-464.

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## See Also

1spls-package, 1 splsCv, plot. 1 spls

## Examples

\#\#FIXME
lsplsCv
Cross-Validate LS-PLS Models

## Description

Calculate cross-validated predictions for LS-PLS models.

## Usage

lsplsCv(formula, ncomp, data, subset, na.action, segments = 10, segment.type = c("random", "consecutive", "interleaved"), length.seg, model = TRUE, ...)

## Arguments

| formula | model formula. See Details. |
| :--- | :--- |
| ncomp | list or vector of positive integers, giving the number of components to use for <br> each PLS matrix. See Details. <br> an optional data frame with the data to fit the model from. <br> an optional vector specifying a subset of observations to be used in the fitting <br> process. <br> a function which indicates what should happen when the data contain missing <br> values. <br> subset |
| na. action | the number of segments to use, or a list with segments (see Details). |
| segments |  |
| segment.type type of segments to use. Ignored if segments is a list. |  |
| length.seg | Positive integer. The length of the segments to use. If specified, it overrides <br> segments unless segments is a list. <br> logical. If TRUE, the model frame is returned. <br> model |
| I. | additional arguments, passed to the underlying cross-validation function (cur- <br> rently orthlsplsCv). |

## Details

The function performs a cross-validation, using the model and segments specified in the call. It returns an object of class "lsplsCv", which has a plot method (see plot.lsplsCv). See lsplspackage for typical usage and more about LS-PLS models.
See lspls for details about specifying the model with formula and ncomp. Note that lsplsCv cross-validates models with from 0 components to the numbers of components specified with ncomp.
If segments is a list, the arguments segment. type and length. seg are ignored. The elements of the list should be integer vectors specifying the indices of the segments. See cvsegments for details.
Otherwise, segments of type segment.type are generated. How many segments to generate is selected by specifying the number of segments in segments, or giving the segment length in length. seg. If both are specified, segments is ignored.

## Value

An object of class "lsplsCv", with components

| pred | the cross-validated predictions. An array with one dimension for the observa- <br> tions, one for the responses, and one for each of the PLS matrices. |
| :--- | :--- |
| segments | the list of segments used in the cross-validation. <br> if observations with missing values were removed, na. action contains a vector <br> na. action <br> with their indices. |
| ncomp | the list of number of components used in the model. |
| call | the function call. |
| terms | the model terms. |
| model | if model $=$ TRUE, the model frame. |

## Note

Currently, lsplsCv handles the formula and the data, and calls orthlsplsCv for the actual crossvalidation. The formula interface is experimental, and might change in future versions.

## Author(s)

Bjørn-Helge Mevik

## References

Jørgensen, K., Segtnan, V. H., Thyholt, K., Næs, T. (2004) A Comparison of Methods for Analysing Regression Models with Both Spectral and Designed Variables. Journal of Chemometrics, 18(10), 451-464.

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## See Also

lspls, plot.lsplsCv, cvsegments, orthlsplsCv, lspls-package

## Examples

\#\#FIXME

MSEP.1splsCv
MSEP, RMSEP and $R^{\wedge} 2$ for $L S-P L S$

## Description

(Root) Mean Squared Error of Prediction ((R)MSEP) and R^2 methods for LS-PLS cross-validations ("lsplsCv" objects).

## Usage

```
## S3 method for class 'lsplsCv'
MSEP(object, scale = FALSE, ...)
    ## S3 method for class 'lsplsCv'
    RMSEP(object, scale = FALSE, ...)
    ## S3 method for class 'lsplsCv'
    R2(object, ...)
```


## Arguments

object an "lsplsCv" object, typically the output from lsplsCv.
scale logical. Whether the responses and predicted values should be divided by the standard deviation of the response prior to calculating the measure. This is most useful when comparing several responses. Default is not to scale. Note that this argument is ignored by the R2 method, since $R^{2}$ is independent of scale.
... Further arguments. Currently unused.

## Value

An array. The first dimension corresponds to the responses (for single-response models, the length of this dimension is 1 ). The rest of the dimensions correspond to the number of components from the PLS matrices.

## Author(s)

Bjørn-Helge Mevik

See Also
lsplsCv, plot.lsplsCv

```
orthlspls.fit
```

Underlying LS-PLS Fit Function

## Description

Fits orthogonalized LS-PLS models.

## Usage

orthlspls.fit(Y, X, Z, ncomp)

## Arguments

$Y$ matrix. Response matrix.
$X \quad$ matrix. The first predictor matrix (typically a design matrix).
Z list. List of predictor matrices.
ncomp list. The number of components to fit from each matrix.

## Details

orthlspls.fit is not meant to be called by the user. It is called by lspls to do the actual fitting. See lspls for details about LS-PLS and ncomp. Each element of the list $Z$ should either be a matrix or a list of matrices.

## Value

A list with components

| coefficients | matrix with the final prediction coefficients |
| :--- | :--- |
| predictors | matrix with variables and scores used in the final regression |
| orthCoefs | list of coefficient generating matrices, to be used when predicting new predic- <br> tors. |
| models | list of fitted PLS models for the matrices |
| ncomp | list with the number of components used |
| scores | list of score matrices |
| loadings | list of loading matrices |
| residuals | matrix with fit residuals, one coloumn per response |

## Note

The interface (arguments and return values) is likely to change in a future version.

## Author(s)

Bjørn-Helge Mevik

## References

Jørgensen, K., Segtnan, V. H., Thyholt, K., Næs, T. (2004) A Comparison of Methods for Analysing Regression Models with Both Spectral and Designed Variables. Journal of Chemometrics, 18(10), 451-464.

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## See Also

lspls

```
orthlsplsCv Low Level Cross-Validation Function
```


## Description

Low-level function to perform the cross-validation in lsplsCv.

## Usage

orthlsplsCv(Y, X, Z, ncomp, segments, trace = FALSE, ...)
orthlsplsCv

## Arguments

| Y | matrix. Response matrix. |
| :--- | :--- |
| X | matrix. The first predictor matrix (typically a design matrix). |
| Z | list. List of predictor matrices. |
| ncomp | list. The number of components to fit from each matrix. |
| segments | list. The segments to use. |
| trace | logical; if TRUE, the segment number is printed for each segment. |
| $\ldots$ | Further arguments. Currently not used. |

## Details

This function is not meant to be called directly by the user. It performs cross-validation of ortogonalized LS-PLS-models without splitting of parallell matrices into common and unique components. See the references for details.

## Value

An array of cross-validated predictions. The first dimension corresponds to the observations, the second to the responses, and the rest to the number of components of the PLS models.

## Author(s)

Bjørn-Helge Mevik

## References

Jørgensen, K., Segtnan, V. H., Thyholt, K., Næs, T. (2004) A Comparison of Methods for Analysing Regression Models with Both Spectral and Designed Variables. Journal of Chemometrics, 18(10), 451-464.

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## See Also

lspls, lsplsCv, orthlspls.fit

## Description

Plot method for "lspls" objects.

## Usage

```
## S3 method for class 'lspls'
    plot(x, plottype = c("scores", "loadings"), ...)
    ## S3 method for class 'lspls'
    scoreplot(object, ...)
    ## S3 method for class 'lspls'
    loadingplot(object, ...)
```


## Arguments

$x$, object Object of class "lspls". The model to be plotted.
plottype character string. What type of plot to generate.
... Further arguments, passed on to underlying plot functions.

## Details

The plot method simply calls scoreplot.lspls or loadingplot.lspls depending on the plottype argument.
scoreplot.lspls gives a series of score plots, one for each PLS model. The user is asked to press Return between each plot.
loadingplot. lspls shows a series of loading plots, one for each PLS model. All plots are shown in the same plot window.

## Value

The functions return whatever the (last) underlying plot function returns.

## Author(s)

Bjørn-Helge Mevik

## See Also

lspls, scoreplot, loadingplot, plot.lsplsCV

## Examples

\#\#FIXME

## Description

Plot method for "lsplsCv" objects. It plots the cross-validated (R)MSEP or R^2 against the total number of components or the matrices included in the model.

## Usage

```
## S3 method for class 'lsplsCv'
plot(x, which = c("RMSEP", "MSEP", "R2"), ncomp,
            separate = TRUE, scale = !isTRUE(separate), ...)
```


## Arguments

x
which character string. Which measure to plot.
ncomp list. The number of components to use when plotting, for each PLS matrix in the model. See Details.
separate logical. Whether separate plots should be generated for each response (default) or one plot with the sum of the measure for all responses.
scale logical. Whether the responses and predicted values should be divided by the standard deviation of the response prior to calculating the measure. Default is to scale when producing a combined plot (separate $=$ FALSE) and not to scale otherwise.
... Further arguments, sent to the underlying plot function.

## Details

If ncomp is not specified, the plot method generates a plot of the cross-validated (R)MSEP or $\mathrm{R}^{\wedge} 2$ values for all combinations of number of components. The values are plotted against the total number of components. Each point is labelled with the combination of number of components. E.g., for a model with three PLS matrices, ' 132 ' means one component from the first matrix, three from the second and two from the third. Also, the lowest (R)MSEP or highest $R^{2}$ values for each total number of components are joined by a line.

If ncomp is specified, the plot method plots (R)MSEP or $\mathrm{R}^{\wedge} 2$ for models with the first matrix, with the two first matrices, etc. ncomp should be specified as when running lsplsCv, and is used for selecting the number of components for each PLS matrix. For instance

```
mod <- lsplsCv(Y ~ X + Z + V:W, ...)
plot(mod, ncomp = list(2, c(1,3)))
```

would plot the RMSEPs for $Y \sim X, Y \sim X+Z$ and $Y \sim X+Z+V: W$, using 2, 1 and 3 components for $\mathrm{Z}, \mathrm{V}$ and W , respectively.
If separate is TRUE, a separate plot panel is produced for each response. Otherwise the measure is added for all responses and shown in one plot. If scale is TRUE (the default when producing a combined plot), the measures for each response are standardised by dividing the responses and predicted values by the standard deviation of the (corresponding) response prior to calculating the measure. Note that scale is ignored when which is "R2" because $R^{2}$ is independent of scale.)

## Value

The function returns whatever the (last) underlying plot function returns.

## Author(s)

Bjørn-Helge Mevik

## See Also

```
lsplsCv, lspls
```


## Examples

\#\#FIXME

```
predict.lspls
```


## Description

Predict method for "lspls" objects. It predicts response values or scores from new data.

## Usage

```
    ## S3 method for class 'lspls'
```

    predict(object, newdata, type = c("response", "scores"),
        na.action = na.pass, ...)
    
## Arguments

object object of class "lspls". The fitted model to predict with.
newdata data frame. The new data.
type character. Wether to predict responses or scores.
na.action function determining what should be done with missing values in newdata. The default is to predict NA. See na.omit for alternatives.
... further arguments. Currently not used.

## Value

If type = "response", a matrix with predicted response values is returned. If type = "scores", a matrix with predicted score values is returned.

## Author(s)

Bjørn-Helge Mevik

## See Also

lspls

## Examples

```
##FIXME
```

projections

Projection and Orthogonalisation

## Description

Functions to project one matrix onto another, or to ortghogonalise it against the other.

## Usage

$\operatorname{project}(M, N)$
$\operatorname{orth}(M, N)$
$\operatorname{Corth}(M, N)$

## Arguments

M
matrix to be projected or orthogonalised
N
matrix to be projected onto or orthogonalised against

## Details

project $(\mathrm{M}, \mathrm{N})$ calculates the projection of M onto N , i.e., $N\left(N^{t} N\right)^{-1} N^{t} M$.
orth (M, N) orthogonalises $M$ with respect to $N$, i.e., it calculates the projection of $M$ onto the orthogonal space of $\mathrm{N}: M-N\left(N^{t} N\right)^{-1} N^{t} M$.
Corth(M, N) calculates the coefficient matrix needed to orthogonalise future matrices, that is, $\left(N^{t} N\right)^{-1} N^{t} M$. Future matrices $m$ and $n$ can be orthogonalised with $m-n \% * \% \operatorname{Corth}(M, N)$.

## Value

A matrix.

## Note

The functions need to be opitmised, both for speed and numerical accurracy.

## Author(s)

Bjørn-Helge Mevik
See Also
lspls, lsplsCv, predict.lspls

## Examples

\#\#FIXME

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