Package ‘pls’

October 1, 2019

Title Partial Least Squares and Principal Component Regression

Version 2.7-2

Date 2019-09-30

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Encoding UTF-8

LazyData yes

Description Multivariate regression methods
   Partial Least Squares Regression (PLSR), Principal Component
   Regression (PCR) and Canonical Powered Partial Least Squares (CPPLS).

Depends R (>= 2.10)

Imports grDevices, graphics, methods, stats

Suggests MASS, parallel, Rmpi, testthat, RUnit

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URL http://mevik.net/work/software/pls.html,
https://github.com/bhmevik/pls

BugReports https://github.com/bhmevik/pls/issues

NeedsCompilation no

Repository CRAN

Date/Publication 2019-10-01 17:30:02 UTC

R topics documented:

   biplot.mvr ................................................. 2
   coef.mvr .................................................. 4
   coefplot .................................................. 6
biplot.mvr

Biplots of PLSR and PCR Models.

Description

Biplot method for mvr objects.

Usage

```r
## S3 method for class 'mvr'
biplot(x, comps = 1:2, which = c("x", "y", "scores", "loadings"),
       var.axes = FALSE, xlabs, ylabs, main, ...)
```
**Arguments**

- **x**: an `mvr` object.
- **comps**: integer vector of length two. The components to plot.
- **which**: character. Which matrices to plot. One of "x" (X scores and loadings), "y" (Y scores and loadings), "scores" (X and Y scores) and "loadings" (X and Y loadings).
- **var.axes**: logical. If TRUE, the second set of points have arrows representing them.
- **xlabs**: either a character vector of labels for the first set of points, or FALSE for no labels. If missing, the row names of the first matrix is used as labels.
- **ylabs**: either a character vector of labels for the second set of points, or FALSE for no labels. If missing, the row names of the second matrix is used as labels.
- **main**: character. Title of plot. If missing, a title is constructed by `biplot.mvr`.
- **...**: Further arguments passed on to `biplot.default`.

**Details**

`biplot.mvr` can also be called through the `mvr` plot method by specifying `plottype = "biplot"`.

**Author(s)**

Ron Wehrens and Bjørn-Helge Mevik

**See Also**

`mvr`, `plot.mvr`, `biplot.default`

**Examples**

```r
data(oliveoil)
mod <- plsr(sensory ~ chemical, data = oliveoil)
## Not run:
## These are equivalent
biplot(mod)
plot(mod, plottype = "biplot")

## The four combinations of x and y points:
par(mfrow = c(2,2))
biplot(mod, which = "x") # Default
biplot(mod, which = "y")
biplot(mod, which = "scores")
biplot(mod, which = "loadings")

## End(Not run)
```
Description

Functions to extract information from mvr objects: Regression coefficients, fitted values, residuals, the model frame, the model matrix, names of the variables and components, and the X variance explained by the components.

Usage

```r
## S3 method for class 'mvr'
coef(object, ncomp = object$ncomp, comps, intercept = FALSE, ...)
## S3 method for class 'mvr'
fitted(object, ...)
## S3 method for class 'mvr'
residuals(object, ...)
## S3 method for class 'mvr'
model.matrix(object, ...)
## S3 method for class 'mvr'
model.frame(formula, ...)
prednames(object, intercept = FALSE)
respnames(object)
compnames(object, comps, explvar = FALSE, ...)
explvar(object)
```

Arguments

- `object, formula` an mvr object. The fitted model.
- `ncomp, comps` vector of positive integers. The components to include in the coefficients or to extract the names of. See below.
- `intercept` logical. Whether coefficients for the intercept should be included. Ignored if `comps` is specified. Defaults to `FALSE`.
- `explvar` logical. Whether the explained X variance should be appended to the component names.
- `...` other arguments sent to underlying functions. Currently only used for `model.frame.mvr` and `model.matrix.mvr`.

Details

These functions are mostly used inside other functions. (Functions `coef.mvr`, `fitted.mvr` and `residuals.mvr` are usually called through their generic functions `coef`, `fitted` and `residuals`, respectively.)
coef.mvr is used to extract the regression coefficients of a model, i.e. the $B$ in $y = XB$ (for the $Q$ in $y = TQ$ where $T$ is the scores, see Yloadings). An array of dimension $c(nxvar, nyvar, length(ncomp))$ or $c(nxvar, nyvar, length(comps))$ is returned.

If `comps` is missing (or is NULL), `coef()[, , ncomp[i]]` are the coefficients for models with `ncomp[i]` components, for $i = 1, ..., length(ncomp)$. Also, if `intercept = TRUE`, the first dimension is $nxvar + 1$, with the intercept coefficients as the first row.

If `comps` is given, however, `coef()[, , comps[i]]` are the coefficients for a model with only the component `comps[i]`, i.e. the contribution of the component `comps[i]` on the regression coefficients.

fitted.mvr and residuals.mvr return the fitted values and residuals, respectively. If the model was fitted with `na.action = na.exclude` (or after setting the default `na.action` to "na.exclude" with `options`), the fitted values (or residuals) corresponding to excluded observations are returned as `NA`; otherwise, they are omitted.

model.frame.mvr returns the model frame; i.e. a data frame with all variables neccessary to generate the model matrix. See `model.frame` for details.

model.matrix.mvr returns the (possibly coded) matrix used as $X$ in the fitting. See `model.matrix` for details.

prednames, respnames and compnames extract the names of the $X$ variables, responses and components, respectively. With `intercept = TRUE` in prednames, the name of the intercept variable (i.e. "(Intercept)") is returned as well. compnames can also extract component names from score and loading matrices. If `explvar = TRUE` in compnames, the explained variance for each component (if available) is appended to the component names. For optimal formatting of the explained variances when not all components are to be used, one should specify the desired components with the argument `comps`.

explvar extracts the amount of $X$ variance (in per cent) explained by each component in the model. It can also handle score and loading matrices returned by `scores` and `loadings`.

Value

- `coef.mvr` returns an array of regression coefficients.
- `fitted.mvr` returns an array with fitted values.
- `residuals.mvr` returns an array with residuals.
- `model.frame.mvr` returns a data frame.
- `model.matrix.mvr` returns the $X$ matrix.
- `prednames`, `respnames` and `compnames` return a character vector with the corresponding names.
- `explvar` returns a numeric vector with the explained variances, or `NULL` if not available.

Author(s)

Ron Wehrens and Bjørn-Helge Mevik

See Also

`mvr, coef, fitted, residuals, model.frame, model.matrix, na.omit`
Examples

data(yarn)
mod <- pcr(density ~ NIR, data = yarn[yarn$train,], ncomp = 5)
B <- coef(mod, ncomp = 3, intercept = TRUE)
## A manual predict method:
stopifnot(drop(B[,1] + yarn$NIR[yarn$train,] %*% B[,-1,]) ==
  drop(predict(mod, ncomp = 3, newdata = yarn[yarn$train,])))

## Note the difference in formatting:
mod2 <- pcr(density ~ NIR, data = yarn[yarn$train,])
compnames(mod2, explvar = TRUE)[1:3]
compnames(mod2, comps = 1:3, explvar = TRUE)

coefplot

Plot Regression Coefficients of PLSR and PCR models

Description

Function to plot the regression coefficients of an mvr object.

Usage

coefplot(object, ncomp = object$ncomp, comps, intercept = FALSE,
  separate = FALSE, se.whiskers = FALSE, nCols, nRows, labels,
  type = "l", lty, lwd = NULL, pch, cex = NULL, col, legendpos,
  xlab = "variable", ylab = "regression coefficient", main,
  pretty.xlabels = TRUE, xlim, ylim,
  ask = nRows * nCols < nPlots && dev.interactive(), ...)

Arguments

object an mvr object. The fitted model.
ncomp, comps vector of positive integers. The components to plot. See coef.mvr for details.
se.parisual logical. If TRUE, coefficients for different model sizes are blotted in separate plots.
se.whiskers logical. If TRUE, whiskers at plus/minus 1 estimated standard error are added to the plot. This is only available if the model was cross-validated with jackknife = TRUE. Also, in the current implementation, intercept must be FALSE, and separate must be TRUE if length(ncomp) > 1.
intercept logical. Whether coefficients for the intercept should be plotted. Ignored if comps is specified. Defaults to FALSE. See coef.mvr for details.
nCols, nRows integer. The number of columns and rows the plots will be laid out in. If not specified, coefplot tries to be intelligent.
labels optional. Alternative x axis labels. See Details.
type character. What type of plot to make. Defaults to "1" (lines). Alternative types include "p" (points) and "b" (both). See plot for a complete list of types.
coefplot

lty  vector of line types (recycled as necessary). Line types can be specified as integers or character strings (see \texttt{par} for the details).

lwd  vector of positive numbers (recycled as necessary), giving the width of the lines.

pch  plot character. A character string or a vector of single characters or integers (recycled as necessary). See \texttt{points} for all alternatives.

cex  numeric vector of character expansion sizes (recycled as necessary) for the plotted symbols.

col  character or integer vector of colors for plotted lines and symbols (recycled as necessary). See \texttt{par} for the details.

legendpos  Legend position. Optional. Ignored if separate is \texttt{TRUE}. If present, a legend is drawn at the given position. The position can be specified symbolically (e.g., \texttt{legendpos = "topright"}). This requires \texttt{R >= 2.1.0}. Alternatively, the position can be specified explicitly (\texttt{legendpos = t(c(x,y))}) or interactively (\texttt{legendpos = locator()}). This only works well for plots of single-response models.

xlab, ylab  titles for \texttt{x} and \texttt{y} axes. Typically character strings, but can be expressions (e.g., \texttt{expression(R^2)}) or lists. See \texttt{title} for details.

main  optional main title for the plot. See Details.

pretty.xlabels  logical. If \texttt{TRUE}, coefplot tries to plot the \texttt{x} labels more nicely. See Details.

xlim, ylim  optional vector of length two, with the \texttt{x} or \texttt{y} limits of the plot.

ask  logical. Whether to ask the user before each page of a plot.

...  Further arguments sent to the underlying plot functions.

\textbf{Details}

c_coefplot handles multiple responses by making one plot for each response. If separate is \texttt{TRUE}, separate plots are made for each combination of model size and response. The plots are laid out in a rectangular fashion.

If \texttt{legendpos} is given, a legend is drawn at the given position (unless separate is \texttt{TRUE}).

The argument \texttt{labels} can be a vector of labels or one of "names" and "numbers". The labels are used as \texttt{x} axis labels. If \texttt{labels} is "names" or "numbers", the variable names are used as labels, the difference being that with "numbers", the variable names are converted to numbers, if possible. Variable names of the forms "number" or "number text" (where the space is optional), are handled.

The argument \texttt{main} can be used to specify the main title of the plot. It is handled in a non-standard way. If there is only one (sub) plot, \texttt{main} will be used as the main title of the plot. If there is more than one (sub) plot, however, the presence of \texttt{main} will produce a corresponding 'global' title on the page. Any graphical parameters, e.g., \texttt{cex.main}, supplied to coefplot will only affect the ordinary plot titles, not the 'global' one. Its appearance can be changed by setting the parameters with \texttt{par}, which will affect both titles. (To have different settings for the two titles, one can override the \texttt{par} settings with arguments to coefplot.)

The argument \texttt{pretty.xlabels} is only used when \texttt{labels} is specified. If \texttt{TRUE} (default), the code tries to use a 'pretty' selection of labels. If \texttt{labels} is "numbers", it also uses the numerical values
of the labels for horizontal spacing. If one has excluded parts of the spectral region, one might therefore want to use `pretty.xlabels = FALSE`.

When `separate` is `TRUE`, the arguments `lty`, `col`, and `pch` default to their `par()` setting. Otherwise, the default for all of them is `1:nLines`, where `nLines` is the number of model sizes specified, i.e., the length of `ncomp` or `comps`.

The function can also be called through the `mvr` plot method by specifying `plottype = "coefficients"`.

Note

`legend` has many options. If you want greater control over the appearance of the legend, omit the `legendpos` argument and call `legend` manually.

The handling of labels and `pretty.xlabels` is experimental.

Author(s)

Ron Wehrens and Bjørn-Helge Mevik

See Also

`mvr`, `plot.mvr`, `coef.mvr`, `plot`, `legend`

Examples

```r
data(yarn)
mod.nir <- plsr(density ~ NIR, ncomp = 8, data = yarn)
## Not run:
coefplot(mod.nir, ncomp = 1:6)
plot(mod.nir, plottype = "coefficients", ncomp = 1:6) # Equivalent to the previous
## Plot with legend:
coefplot(mod.nir, ncom = 1:6, legendpos = "bottomright")
## End(Not run)

data(oliveoil)
mod.sens <- plsr(sensory ~ chemical, ncomp = 4, data = oliveoil)
## Not run: coefplot(mod.sens, ncomp = 2:4, separate = TRUE)
```

Description

Fits a PLS model using the CPPLS algorithm.

Usage

```r
cppls.fit(X, Y, ncomp, Y.add = NULL, center = TRUE,
stripped = FALSE, lower = 0.5, upper = 0.5,
trunc.pow = FALSE, weights = NULL, ...)
```
Arguments

- **X**: a matrix of observations. NAs and Inf's are not allowed.
- **Y**: a vector or matrix of responses. NAs and Inf's are not allowed.
- **ncomp**: the number of components to be used in the modelling.
- **Y.add**: a vector or matrix of additional responses containing relevant information about the observations.
- **center**: logical, determines if the X and Y matrices are mean centered or not. Default is to perform mean centering.
- **stripped**: logical. If TRUE the calculations are stripped as much as possible for speed; this is meant for use with cross-validation or simulations when only the coefficients are needed. Defaults to FALSE.
- **lower**: a vector of lower limits for power optimisation. Defaults to 0.5.
- **upper**: a vector of upper limits for power optimisation. Defaults to 0.5.
- **trunc.pow**: logical. If TRUE an experimental alternative power algorithm is used. (Optional)
- **weights**: a vector of individual weights for the observations. (Optional)
- ... other arguments. Currently ignored.

Details

This function should not be called directly, but through the generic functions cppls or mvr with the argument method="cppls". Canonical Powered PLS (CPPLS) is a generalisation of PLS incorporating discrete and continuous responses (also simultaneously), additional responses, individual weighting of observations and power methodology for sharpening focus on groups of variables. Depending on the input to cppls it can produce the following special cases:

- PLS: uni-response continuous Y
- PPLS: uni-response continuous Y, (lower || upper) != 0.5
- PLS-DA (using correlation maximisation - B/W): dummy-coded discrete response Y
- PPLS-DA: dummy-coded discrete response Y, (lower || upper) != 0.5
- CPLS: multi-response Y (continuous, discrete or combination)
- CPPLS: multi-response Y (continuous, discrete or combination), (lower || upper) != 0.5

The name "canonical" comes from canonical correlation analysis which is used when calculating vectors of loading weights, while "powered" refers to a reparameterisation of the vectors of loading weights which can be optimised over a given interval.

Value

A list containing the following components is returned:

- **coefficients**: an array of regression coefficients for 1, ..., ncomp components. The dimensions of coefficients are c(nvar,npred,ncomp) with nvar the number of X variables and npred the number of variables to be predicted in Y.
- **scores**: a matrix of scores.
loadings a matrix of loadings.
loading.weights a matrix of loading weights.
Yscores a matrix of Y-scores.
Yloadings a matrix of Y-loadings.
projection the projection matrix used to convert X to scores.
Xmeans a vector of means of the X variables.
Ymeans a vector of means of the Y variables.
fitted.values an array of fitted values. The dimensions of fitted.values are c(nobj,npred,ncomp) with nobj the number samples and npred the number of Y variables.
residuals an array of regression residuals. It has the same dimensions as fitted.values.
Xvar a vector with the amount of X-variance explained by each component.
Xtotvar total variance in X.
gammas gamma-values obtained in power optimisation.
canonical.correlations Canonical correlation values from the calculations of loading weights.
A matrix containing vectors of weights a from canonical correlation (cor(Za,Yb)).
smallNorms vector of indices of explanatory variables of length close to or equal to 0.

If stripped is TRUE, only the components coefficients, Xmeans, Ymeans and gammas are returned.

Author(s)
Kristian Hovde Liland

References

See Also
mvr plsr pcr widekernelpls.fit simpls.fit oscorespls.fit

Examples

data(mayonnaise)
# Create dummy response
mayonnaise$dummy <-
  I(model.matrix(~y-1, data.frame(y = factor(mayonnaise$oil.type))))
# Predict CPLS scores for test data
may.cpls <- cppls(dummy ~ NIR, 10, data = mayonnaise, subset = train)
may.test <- predict(may.cpls, newdata = mayonnaise[!mayonnaise$train,], type = "score")

# Predict CPLS scores for test data (experimental used design as additional Y information)
may.cpls.yadd <- cppls(dummy ~ NIR, 10, data = mayonnaise, subset = train, Y.add=design)
may.test.yadd <- predict(may.cpls.yadd, newdata = mayonnaise[!mayonnaise$train,], type = "score")

# Classification by linear discriminant analysis (LDA)
library(MASS)
error <- matrix(ncol = 10, nrow = 2)
dimnames(error) <- list(Model = c('CPLS', 'CPLS (Y.add)'), ncomp = 1:10)
for (i in 1:10) {
  fitdata1 <- data.frame(oil.type = mayonnaise$oil.type[mayonnaise$train],
      NIR.score = I(may.cpls$scores[,1:i,drop=FALSE]))
  testdata1 <- data.frame(oil.type = mayonnaise$oil.type[!mayonnaise$train],
      NIR.score = I(may.test[,1:i,drop=FALSE]))
  error[1,i] <-
    (42 - sum(predict(lda(oil.type ~ NIR.score, data = fitdata1),
                  newdata = testdata1$oil.type) == testdata1$oil.type)) / 42
  fitdata2 <- data.frame(oil.type = mayonnaise$oil.type[mayonnaise$train],
      NIR.score = I(may.cpls.yadd$scores[,1:i,drop=FALSE]))
  testdata2 <- data.frame(oil.type = mayonnaise$oil.type[!mayonnaise$train],
      NIR.score = I(may.test.yadd[,1:i,drop=FALSE]))
  error[2,i] <-
    (42 - sum(predict(lda(oil.type ~ NIR.score, data = fitdata2),
                  newdata = testdata2$oil.type) == testdata2$oil.type)) / 42
}
round(error,2)

crossval

Cross-validation of PLSR and PCR models

Description

A “stand alone” cross-validation function for mvr objects.

Usage

crossval(object, segments = 10,
  segment.type = c("random", "consecutive", "interleaved"),
  length.seg, jackknife = FALSE, trace = 15, ...)

Arguments

object an mvr object; the regression to cross-validate.
segments the number of segments to use, or a list with segments (see below).
segment.type the type of segments to use. Ignored if segments is a list.
**Details**

This function performs cross-validation on a model fit by mvr. It can handle models such as `plsr(y ~ msc(X),...)` or other models where the predictor variables need to be recalculated for each segment. When recalculation is not needed, the result of `crossval(mvr(...))` is identical to `mvr(...,validation = "CV")`, but slower.

Note that to use `crossval`, the data **must** be specified with a `data` argument when fitting object.

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.

If `jackknife` is `TRUE`, jackknifed regression coefficients are returned, which can be used for for variance estimation (`var.jack`) or hypothesis testing (`jack.test`).

When tracing is turned on, the segment number is printed for each segment.

By default, the cross-validation will be performed serially. However, it can be done in parallel using functionality in the `parallel` package by setting the option `parallel` in `pls.options`. See `pls.options` for the different ways to specify the parallelism. See also Examples below.

**Value**

The supplied object is returned, with an additional component `validation`, which is a list with components

- `method`: euqals "CV" for cross-validation.
- `pred`: an array with the cross-validated predictions.
- `coefficients`: (only if `jackknife` is TRUE) an array with the jackknifed regression coefficients. The dimensions correspond to the predictors, responses, number of components, and segments, respectively.
- `PRESS0`: a vector of PRESS values (one for each response variable) for a model with zero components, i.e., only the intercept.
- `PRESS`: a matrix of PRESS values for models with 1, ..., `ncomp` components. Each row corresponds to one response variable.
- `adj`: a matrix of adjustment values for calculating bias corrected MSEP. MSEP uses this.
- `segments`: the list of segments used in the cross-validation.
ncomp

gammas

the number of components.

if method cppls is used, gamma values for the powers of each CV segment are returned.

Note

The PRESS0 is always cross-validated using leave-one-out cross-validation. This usually makes little difference in practice, but should be fixed for correctness.

The current implementation of the jackknife stores all jackknife-replicates of the regression coefficients, which can be very costly for large matrices. This might change in a future version.

Author(s)

Ron Wehrens and Bjørn-Helge Mevik

References


See Also

mvr mvrCv cvsegments MSEP var.jack jack.test

Examples

data(yarn)
yarn.pcr <- pcr(density ~ msc(NIR), 6, data = yarn)
yarn.cv <- crossval(yarn.pcr, segments = 10)
## Not run: plot(MSEP(yarn.cv))

## Not run:
## Parallelised cross-validation, using transient cluster:
pls.options(parallel = 4) # use mclapply (not available on Windows)
pls.options(parallel = quote(parallel::makeCluster(4, type = "PSOCK"))) # parLapply
## A new cluster is created and stopped for each cross-validation:
yarn.cv <- crossval(yarn.pcr)
yarn.loocv <- crossval(yarn.pcr, length.seg = 1)

## Parallelised cross-validation, using persistent cluster:
library(parallel)
## This creates the cluster:
pls.options(parallel = makeCluster(4, type = "FORK")) # not available on Windows
pls.options(parallel = makeCluster(4, type = "PSOCK"))
## The cluster can be used several times:
yarn.cv <- crossval(yarn.pcr)
yarn.loocv <- crossval(yarn.pcr, length.seg = 1)
## The cluster should be stopped manually afterwards:
stopCluster(pls.options()$parallel)
## Parallelised cross-validation, using persistent MPI cluster:
## This requires the packages snow and Rmpi to be installed
library(parallel)
## This creates the cluster:
pls.options(parallel = makeCluster(4, type = "MPI"))
## The cluster can be used several times:
yarn.cv <- crossval(yarn.pcr)
yarn.loocv <- crossval(yarn.pcr, length.seg = 1)
## The cluster should be stopped manually afterwards:
stopCluster(pls.options()$parallel)
## It is good practice to call mpi.exit() or mpi.quit() afterwards:
mpi.exit()
## End(Not run)

---

cvsegments

### Generate segments for cross-validation

#### Description

The function generates a list of segments for cross-validation. It can generate random, consecutive and interleaved segments, and supports keeping replicates in the same segment.

#### Usage

```
cvsegments(N, k, length.seg = ceiling(N / k), nrep = 1,
            type = c("random", "consecutive", "interleaved"))
```

#### Arguments

- **N**: Integer. The number of rows in the data set.
- **k**: Integer. The number of segments to return.
- **length.seg**: Integer. The length of the segments. If given, it overrides k.
- **nrep**: Integer. The number of (consecutive) rows that are replicates of the same object. Replicates will always be kept in the same segment.
- **type**: One of "random", "consecutive" and "interleaved". The type of segments to generate. Default is "random".

#### Details

If `length.seg` is specified, it is used to calculate the number of segments to generate. Otherwise `k` must be specified. If $k \times length.seg \neq N$, the $k \times length.seg - N$ last segments will contain only $length.seg - 1$ indices.

If `type` is "random", the indices are allocated to segments in random order. If it is "consecutive", the first segment will contain the first $length.seg$ indices, and so on. If `type` is "interleaved", the first segment will contain the indices $1, length.seg + 1, 2 \times length.seg + 1, \ldots, (k - 1) \times length.seg + 1$, and so on.
If \( n_{rep} > 1 \), it is assumed that each \( n_{rep} \) consecutive rows are replicates (repeated measurements) of the same object, and care is taken that replicates are never put in different segments.

Warning: If \( k \) does not divide \( N \), a specified \( length\_seg \) does not divide \( N \), or \( n_{rep} \) does not divide \( length\_seg \), the number of segments and/or the segment length will be adjusted as needed. Warnings are printed for some of these cases, and one should always inspect the resulting segments to make sure they are as expected.

**Value**

A list of vectors. Each vector contains the indices for one segment. The attribute "incomplete" contains the number of incomplete segments, and the attribute "type" contains the type of segments.

**Author(s)**

Bjørn-Helge Mevik and Ron Wehrens

**Examples**

```r
## Segments for 10-fold randomised cross-validation:
CVsegments(100, 10)

## Segments with four objects, taken consecutive:
CVsegments(60, length.seg = 4, type = "cons")

## Incomplete segments
segs <- CVsegments(50, length.seg = 3)
attr(segs, "incomplete")

## Leave-one-out cross-validation:
CVsegments(100, 100)

## Leave-one-out with variable/unknown data set size \( n \):
n <- 50
CVsegments(n, length.seg = 1)

## Data set with replicates
CVsegments(100, 25, nrep = 2)

## Note that rows 1 and 2 are in the same segment, rows 3 and 4 in the same segment, and so on.
```

---

**Description**

A data set with NIR spectra and octane numbers of 60 gasoline samples. The NIR spectra were measured using diffuse reflectance as \( \log(1/R) \) from 900 nm to 1700 nm in 2 nm intervals, giving 401 wavelengths. Many thanks to John H. Kalivas.

---

**gasoline**

*Octane numbers and NIR spectra of gasoline*
Usage
gasoline

Format
A data frame with 60 observations on the following 2 variables.

octane a numeric vector. The octane number.
NIR a matrix with 401 columns. The NIR spectrum.

Source

jack.test

Jackknife approximate t tests of regression coefficients

Description
Performes approximate t tests of regression coefficients based on jackknife variance estimates.

Usage
jack.test(object, ncomp = object$ncomp, use.mean = TRUE)
## S3 method for class 'jacktest'
print(x, P.values = TRUE, ...)

Arguments
object an mvr object. A cross-validated model fitted with jackknife = TRUE.
ncomp the number of components to use for estimating the variances
use.mean logical. If TRUE (default), the mean coefficients are used when estimating the (co)variances; otherwise the coefficients from a model fitted to the entire data set. See var.jack for details.
x an jacktest object, the result of jack.test.
P.values logical. Whether to print p values (default).
... Further arguments sent to the underlying print function printCoefmat.

Details
jack.test uses the variance estimates from var.jack to perform t tests of the regression coefficients. The resulting object has a print method, print.jacktest, which uses printCoefmat for the actual printing.
Value

jack.test returns an object of class "jacktest", with components

- coefficients: The estimated regression coefficients
- sd: The square root of the jackknife variance estimates
- tvalues: The \( t \) statistics
- df: The 'degrees of freedom' used for calculating \( p \) values
- pvalues: The calculated \( p \) values

print.jacktest returns the "jacktest" object (invisibly).

Warning

The jackknife variance estimates are known to be biased (see var.jack). Also, the distribution of the regression coefficient estimates and the jackknife variance estimates are unknown (at least in PLSR/PCR). Consequently, the distribution (and in particular, the degrees of freedom) of the resulting \( t \) statistics is unknown. The present code simply assumes a \( t \) distribution with \( m - 1 \) degrees of freedom, where \( m \) is the number of cross-validation segments.

Therefore, the resulting \( p \) values should not be used uncritically, and should perhaps be regarded as mere indicator of (non-)significance.

Finally, also keep in mind that as the number of predictor variables increase, the problem of multiple tests increases correspondingly.

Author(s)

Bjørn-Helge Mevik

References


See Also

var.jack, mvrCv

Examples

data(oliveoil)
mod <- pcr(sensory ~ chemical, data = oliveoil, validation = "LOO", jackknife = TRUE)
jack.test(mod, ncomp = 2)
kernelpls.fit  

*Kernel PLS (Dayal and MacGregor)*

**Description**

Fits a PLSR model with the kernel algorithm.

**Usage**

```
kernelpls.fit(X, Y, ncomp, center = TRUE, stripped = FALSE, ...)
```

**Arguments**

- `X`  
a matrix of observations. NAs and Infs are not allowed.
- `Y`  
a vector or matrix of responses. NAs and Infs are not allowed.
- `ncomp`  
the number of components to be used in the modelling.
- `center`  
logical, determines if the `X` and `Y` matrices are mean centered or not. Default is to perform mean centering.
- `stripped`  
logical. If `TRUE` the calculations are stripped as much as possible for speed; this is meant for use with cross-validation or simulations when only the coefficients are needed. Defaults to `FALSE`.
- `...`  
other arguments. Currently ignored.

**Details**

This function should not be called directly, but through the generic functions `plsr` or `mvr` with the argument `method="kernelpls"` (default). Kernel PLS is particularly efficient when the number of objects is (much) larger than the number of variables. The results are equal to the NIPALS algorithm. Several different forms of kernel PLS have been described in literature, e.g. by De Jong and Ter Braak, and two algorithms by Dayal and MacGregor. This function implements the fastest of the latter, not calculating the crossproduct matrix of `X`. In the Dyal & MacGregor paper, this is “algorithm 1”.

**Value**

A list containing the following components is returned:

- `coefficients`  
an array of regression coefficients for 1, ..., `ncomp` components. The dimensions of coefficients are `c(nvar, npred, ncomp)` with `nvar` the number of `X` variables and `npred` the number of variables to be predicted in `Y`.
- `scores`  
a matrix of scores.
- `loadings`  
a matrix of loadings.
- `loading.weights`  
a matrix of loading weights.
- `Yscores`  
a matrix of `Y`-scores.
Mayonnaise NIR measurements and oil types of mayonnaise

Yloadings  a matrix of Y-loadings.
projection the projection matrix used to convert X to scores.
Xmeans  a vector of means of the X variables.
Ymeans  a vector of means of the Y variables.
fitted.values an array of fitted values. The dimensions of fitted.values are c(nobj,npred,ncomp) with nobj the number samples and npred the number of Y variables.
residuals an array of regression residuals. It has the same dimensions as fitted.values.
Xvar  a vector with the amount of X-variance explained by each component.
Xtotvar Total variance in X.

If stripped is TRUE, only the components coefficients, Xmeans and Ymeans are returned.

Author(s)
Ron Wehrens and Bjørn-Helge Mevik

References


See Also

mvr plsr cppls pcr widekernelpls.fit simpls.fit oscorespls.fit

---

Data

**Description**

Raw NIR measurements (351 wavelengths, 1100-2500 nm in steps of 4 nm) taken on 54 samples of mayonnaise based on six different oil types (soybean, sunflower, canola, olive, corn, and grapeseed). The resulting 54 samples were measured in triplicates, resulting in 54 x 3 = 162 different spectra (120/42 training/test).

**Usage**

data(mayonnaise)
Format

A data frame with 162 observations on the following 4 variables.

NIR  a matrix with 351 columns
oil.type  a numeric vector
design  a matrix with 5 columns
train  a logical vector

Source


---

**msc**

Multiplicative Scatter Correction

Description

Performs multiplicative scatter/signal correction on a data matrix.

Usage

```r
msc(X, reference = NULL)
## S3 method for class 'msc'
predict(object, newdata, ...)
## S3 method for class 'msc'
makepredictcall(var, call)
```

Arguments

- `X`, `newdata` numeric matrices. The data to scatter correct.
- `reference` numeric vector. Spectre to use as reference. If NULL, the column means of `X` are used.
- `object` an object inheriting from class "msc", normally the result of a call to `msc` with a single matrix argument.
- `var` A variable.
- `call` The term in the formula, as a call.
- `...` other arguments. Currently ignored.

Details

`makepredictcall.msc` is an internal utility function; it is not meant for interactive use. See `makepredictcall` for details.
Value

Both `msc` and `predict.msc` return a multiplicative scatter corrected matrix, with attribute "reference" the vector used as reference spectre. The matrix is given class c("msc","matrix"). For `predict.msc`, the "reference" attribute of object is used as reference spectre.

Author(s)

Bjørn-Helge Mevik and Ron Wehrens

References


See Also

`mvr`, `pcr`, `pls`, `stdize`

Examples

```r
data(yarn)
## Direct correction:
Ztrain <- msc(yarn$NIR[yarn$train,])
Ztest <- predict(Ztrain, yarn$NIR[!yarn$train,])

## Used in formula:
mod <- plsr(density ~ msc(NIR), ncomp = 6, data = yarn[yarn$train,])
pred <- predict(mod, newdata = yarn[!yarn$train,]) # Automatically scatter corrected
```

---

**mvr**

Partial Least Squares and Principal Component Regression

Description

Functions to perform partial least squares regression (PLSR), canonical powered partial least squares (CPPLS) or principal component regression (PCR), with a formula interface. Cross-validation can be used. Prediction, model extraction, plot, print and summary methods exist.

Usage

```r
mvr(formula, ncomp, Y.add, data, subset, na.action,
    method = pls.options()$mvralg,
    scale = FALSE, center = TRUE, validation = c("none", "CV", "LOO"),
    model = TRUE, x = FALSE, y = FALSE, ...)
plsr(..., method = pls.options()$plsralg)
cppls(..., Y.add, weights, method = pls.options()$cpplsalg)
pcr(..., method = pls.options()$pcralg)
```
Arguments

formula: a model formula. Most of the `lm` formula constructs are supported. See below.
ncomp: the number of components to include in the model (see below).
Y.add: a vector or matrix of additional responses containing relevant information about the observations. Only used for `cppls`.
data: an optional data frame with the data to fit the model from.
subset: a function which indicates what should happen when the data contain missing values. The default is set by the `na.action` setting of `options`, and is `na.fail` if that is unset. The ‘factory-fresh’ default is `na.omit`. Another possible value is `NULL`, no action. Value `na.exclude` can be useful. See `na.omit` for other alternatives.
na.action: a function which indicates what should happen when the data contain missing values. The default is set by the `na.action` setting of `options`, and is `na.fail` if that is unset. The ‘factory-fresh’ default is `na.omit`. Another possible value is `NULL`, no action. Value `na.exclude` can be useful. See `na.omit` for other alternatives.
method: the multivariate regression method to be used. If "model.frame", the model frame is returned.
scale: numeric vector, or logical. If numeric vector, $X$ is scaled by dividing each variable with the corresponding element of `scale`. If `scale` is `TRUE`, $X$ is scaled by dividing each variable by its sample standard deviation. If cross-validation is selected, scaling by the standard deviation is done for every segment.
center: logical, determines if the $X$ and $Y$ matrices are mean centered or not. Default is to perform mean centering.
validation: character. What kind of (internal) validation to use. See below.
model: a logical. If `TRUE`, the model frame is returned.
x: a logical. If `TRUE`, the model matrix is returned.
y: a logical. If `TRUE`, the response is returned.
weights: a vector of individual weights for the observations. Only used for `cppls` (Optional)
...: additional optional arguments, passed to the underlying fit functions, and `mvrCv`.

Currently, the fit functions `oscorespls.fit` and `widekernelpls.fit` implement these extra arguments:

tol: numeric. Tolerance used for determining convergence.
maxit: positive integer. The maximal number of iterations used.
and `cppls.fit` implements:
lower: a vector of lower limits for power optimisation.
upper: a vector of upper limits for power optimisation.
trunc.pow: logical. Whether to use an experimental alternative power algorithm.
`mvrCv` implements several arguments; the following are probably the most useful of them:
segments: the number of segments to use, or a list with segments.
segment.type: the type of segments to use.
length.seg: Positive integer. The length of the segments to use.
jackknife: logical. Whether to perform jackknifing of regression coefficients. See the functions’ documentation for details.
Details

The functions fit PLSR, CPPLS or PCR models with 1, ..., ncomp number of components. Multi-
response models are fully supported.

The type of model to fit is specified with the method argument. Four PLSR algorithms are avail-
able: the kernel algorithm ("kernelpls"), the wide kernel algorithm ("widekernelpls"), SIMPLS
("simpls") and the classical orthogonal scores algorithm ("oscorespls"). One CPPLS algorithm
is available ("cppls") providing several extensions to PLS. One PCR algorithm is available: using
the singular value decomposition ("svdpc"). If method is "model.frame", the model frame
is returned. The functions pcr, plsr and cppls are wrappers for mvr, with different values for
method.

The formula argument should be a symbolic formula of the form response ~ terms, where response
is the name of the response vector or matrix (for multi-response models) and terms is the name
of one or more predictor matrices, usually separated by +, e.g., water ~ FTIR or y ~ X + Z. See
lm for a detailed description. The named variables should exist in the supplied data data frame
or in the global environment. Note: Do not use mvr(mydata$y ~ mydata$X,...), instead use
mvr(y ~ X,data = mydata,...). Otherwise, predict.mvr will not work properly. The chapter
‘Statistical models in R’ of the manual ‘An Introduction to R’ distributed with R is a good
reference on formulas in R.

The number of components to fit is specified with the argument ncomp. It this is not supplied, the
maximal number of components is used (taking account of any cross-validation).

All implemented algorithms mean-center both predictor and response matrices. This can be turned
off by specifying center = FALSE. See Seasholtz and Kowalski for a discussion about centering in
PLS regression.

If validation = "CV", cross-validation is performed. The number and type of cross-validation
segments are specified with the arguments segments and segment.type. See mvrCv for details.
If validation = "LOO", leave-one-out cross-validation is performed. It is an error to specify the
segments when validation = "LOO" is specified.

By default, the cross-validation will be performed serially. However, it can be done in parallel
using functionality in the parallel package by setting the option parallel in pls.options. See
pls.options for the different ways to specify the parallelism. See also Examples below.

Note that the cross-validation is optimised for speed, and some generality has been sacrificed. Es-
specially, the model matrix is calculated only once for the complete cross-validation, so models like
y ~ msc(X) will not be properly cross-validated. However, scaling requested by scale = TRUE is
properly cross-validated. For proper cross-validation of models where the model matrix must be
updated/regenerated for each segment, use the separate function crossval.

Value

If method = "model.frame", the model frame is returned. Otherwise, an object of class mvr is
returned. The object contains all components returned by the underlying fit function. In addition, it
contains the following components:

validation if validation was requested, the results of the cross-validation. See mvrCv for
details.

fit.time the elapsed time for the fit. This is used by crossval to decide whether to turn
on tracing.
na.action if observations with missing values were removed, na.action contains a vector with their indices. The class of this vector is used by functions like fitted to decide how to treat the observations.

ncomp the number of components of the model.

method the method used to fit the model. See the argument method for possible values.

scale if scaling was requested (with scale), the scaling used.

call the function call.

terms the model terms.

model if model = TRUE, the model frame.

x if x = TRUE, the model matrix.

y if y = TRUE, the model response.

Author(s)
Ron Wehrens and Bjørn-Helge Mevik

References


See Also
kernelpls.fit, widekernelpls.fit, simpls.fit, oscorespls.fit, cplls.fit, svdpc.fit, mvrCv, crossval, loadings, scores, loading.weights, coef.mvr, predict.mvr, R2, MSEP, RMSEP, plot.mvr

Examples

data(yarn)
## Default methods:
yarn.pcr <- pcr(density ~ NIR, 6, data = yarn, validation = "CV")
yarn.pls <- pls(density ~ NIR, 6, data = yarn, validation = "CV")
yarn.cplls <- cplls(density ~ NIR, 6, data = yarn, validation = "CV")

## Alternative methods:
yarn.oscorespls <- mvr(density ~ NIR, 6, data = yarn, validation = "CV",

method = "oscorespls")
yarn.simpls <- mvr(density ~ NIR, 6, data = yarn, validation = "CV",

method = "simpls")

## Not run:
## Parallelised cross-validation, using transient cluster:
pls.options(parallel = 4) # use mclapply
pls.options(parallel = quote(makeCluster(4, type = "PSOCK"))) # use parLapply
## A new cluster is created and stopped for each cross-validation:
yarn.pls <- pls(density ~ NIR, 6, data = yarn, validation = "CV")
mvrCv <- pcr(density ~ NIR, 6, data = yarn, validation = "CV")

## Parallelised cross-validation, using persistent cluster:
library(parallel)
## This creates the cluster:
pls.options(parallel = makeCluster(4, type = "PSOCK"))
## The cluster can be used several times:
yarn.pls <- plsr(density ~ NIR, 6, data = yarn, validation = "CV")
yarn.pcr <- pcr(density ~ NIR, 6, data = yarn, validation = "CV")
## The cluster should be stopped manually afterwards:
stopCluster(pls.options()$parallel)

## Parallelised cross-validation, using persistent MPI cluster:
## This requires the packages snow and Rmpi to be installed
library(parallel)
## This creates the cluster:
pls.options(parallel = makeCluster(4, type = "MPI"))
## The cluster can be used several times:
yarn.pls <- plsr(density ~ NIR, 6, data = yarn, validation = "CV")
yarn.pcr <- pcr(density ~ NIR, 6, data = yarn, validation = "CV")
## The cluster should be stopped manually afterwards:
stopCluster(pls.options()$parallel)
## It is good practice to call mpi.exit() or mpi.quit() afterwards:
mpi.exit()

## End(Not run)

## Multi-response models:
data(oliveoil)
sens.pcr <- pcr(sensory ~ chemical, ncomp = 4, scale = TRUE, data = oliveoil)
sens.pls <- plsr(sensory ~ chemical, ncomp = 4, scale = TRUE, data = oliveoil)

## Classification
# A classification example utilizing additional response information
# (Y.add) is found in the cppls.fit manual ('See also' above).

---

**mvrCv**

**Cross-validation**

**Description**

Performs the cross-validation calculations for mvr.

**Usage**

mvrCv(X, Y, ncomp, Y.add = NULL, weights = NULL,
      method = pls.options()$mvralg, scale = FALSE,
      segments = 10, segment.type = c("random", "consecutive", "interleaved"),
      length.seg, jackknife = FALSE, trace = FALSE, ...)

## Description

The `mvrCv` function performs cross-validation for the MVR (Multi-Variate Regression) model. It calculates the cross-validation results for a specified number of components (`ncomp`) and different cross-validation methods. The function allows for parallel and MPI-based cross-validation techniques, which can be specified using the `parallel` and `type` arguments of the `pls.options` function.

## Usage

The `mvrCv` function is used as follows:

```r
mvrCv(X, Y, ncomp, Y.add = NULL, weights = NULL,
      method = pls.options()$mvralg, scale = FALSE,
      segments = 10, segment.type = c("random", "consecutive", "interleaved"),
      length.seg, jackknife = FALSE, trace = FALSE, ...)
```

- **X**: The data matrix containing the predictor variables.
- **Y**: The response matrix.
- **ncomp**: The number of components to be used in the model.
- **Y.add**: Additional response data.
- **weights**: Weights for the observations.
- **method**: The method for cross-validation, specified using `pls.options()$mvralg`.
- **scale**: Whether to scale the data.
- **segments**: The number of segments for cross-validation.
- **segment.type**: The type of cross-validation segments.
- **length.seg**: The length of each segment.
- **jackknife**: Whether to use the jackknife method.
- **trace**: Whether to print progress information.

## Examples

### Parallelised Cross-Validation

```r
library(parallel)
pls.options(parallel = makeCluster(4, type = "PSOCK"))

yarn.pls <- plsr(density ~ NIR, 6, data = yarn, validation = "CV")
yarn.pcr <- pcr(density ~ NIR, 6, data = yarn, validation = "CV")

stopCluster(pls.options()$parallel)
```

### Parallelised MPI Cross-Validation

```r
library(parallel)
pls.options(parallel = makeCluster(4, type = "MPI"))

yarn.pls <- plsr(density ~ NIR, 6, data = yarn, validation = "CV")
yarn.pcr <- pcr(density ~ NIR, 6, data = yarn, validation = "CV")

stopCluster(pls.options()$parallel)
```

### Multi-Response Models

```r
data(oliveoil)
sens.pcr <- pcr(sensory ~ chemical, ncomp = 4, scale = TRUE, data = oliveoil)
sens.pls <- plsr(sensory ~ chemical, ncomp = 4, scale = TRUE, data = oliveoil)
```

### Classification

```r
# A classification example utilizing additional response information
# (Y.add) is found in the cppls.fit manual ('See also' above).
```
Arguments

X
a matrix of observations. NAs and Inf$s are not allowed.

Y
a vector or matrix of responses. NAs and Inf$s are not allowed.

ncomp
the number of components to be used in the modelling.

Y.add
a vector or matrix of additional responses containing relevant information about the observations. Only used for cppls.

weights
a vector of individual weights for the observations. Only used for cppls. (Optional)

method
the multivariate regression method to be used.

scale
logical. If TRUE, the learning X data for each segment is scaled by dividing each variable by its sample standard deviation. The prediction data is scaled by the same amount.

segments
the number of segments to use, or a list with segments (see below).

segment.type
the 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 segments unless segments is a list.

jackknife
logical. Whether jackknifing of regression coefficients should be performed.

trace
logical; if TRUE, the segment number is printed for each segment.

... additional arguments, sent to the underlying fit function.

Details

This function is not meant to be called directly, but through the generic functions pcr, plsr, cppls or mvr with the argument validation set to "CV" or "LOO". All arguments to mvrCv can be specified in the generic function call.

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.

If jackknife is TRUE, jackknifed regression coefficients are returned, which can be used for for variance estimation (var.jack) or hypothesis testing (jack.test).

X and Y do not need to be centered.

Note that this function cannot be used in situations where X needs to be recalculated for each segment (except for scaling by the standard deviation), for instance with msc or other preprocessing. For such models, use the more general (but slower) function crossval.

Also note that if needed, the function will silently(!) reduce ncomp to the maximal number of components that can be cross-validated, which is $n - l - 1$, where $n$ is the number of observations and $l$ is the length of the longest segment. The (possibly reduced) number of components is returned as the component ncomp.

By default, the cross-validation will be performed serially. However, it can be done in parallel using functionality in the parallel package by setting the option parallel in pls.options. See pls.options for the different ways to specify the parallelism.
Value

A list with the following components:

- **method**: equals "CV" for cross-validation.
- **pred**: an array with the cross-validated predictions.
- **coefficients**: (only if `jackknife` is TRUE) an array with the jackknifed regression coefficients. The dimensions correspond to the predictors, responses, number of components, and segments, respectively.
- **PRESS0**: a vector of PRESS values (one for each response variable) for a model with zero components, i.e., only the intercept.
- **PRESS**: a matrix of PRESS values for models with 1, \ldots, `ncomp` components. Each row corresponds to one response variable.
- **adj**: a matrix of adjustment values for calculating bias corrected MSEP. MSEP uses this.
- **segments**: the list of segments used in the cross-validation.
- **ncomp**: the actual number of components used.
- **gamma**: if method `cppls` is used, gamma values for the powers of each CV segment are returned.

Note

The PRESS0 is always cross-validated using leave-one-out cross-validation. This usually makes little difference in practice, but should be fixed for correctness.

The current implementation of the jackknife stores all jackknife-replicates of the regression coefficients, which can be very costly for large matrices. This might change in a future version.

Author(s)

Ron Wehrens and Bjørn-Helge Mevik

References


See Also

- `mvr`, `crossval`, `cvsegments`, `MSEP`, `var.jack`, `jack.test`

Examples

```r
data(yarn)
yarn.pcr <- pcr(density ~ NIR, 6, data = yarn, validation = "CV", segments = 10)
## Not run: plot(MSEP(yarn.pcr))
```
Description

Functions to estimate the mean squared error of prediction (MSEP), root mean squared error of prediction (RMSEP) and $R^2$ (A.K.A. coefficient of multiple determination) for fitted PCR and PLSR models. Test-set, cross-validation and calibration-set estimates are implemented.

Usage

MSEP(object, ...)  
## S3 method for class 'mvr'  
MSEP(object, estimate, newdata, ncomp = 1:object$ncomp, comps,  
    intercept = cumulative, se = FALSE, ...)

RMSEP(object, ...)  
## S3 method for class 'mvr'  
RMSEP(object, ...)  

R2(object, ...)  
## S3 method for class 'mvr'  
R2(object, estimate, newdata, ncomp = 1:object$ncomp, comps,  
    intercept = cumulative, se = FALSE, ...)

mvrValstats(object, estimate, newdata, ncomp = 1:object$ncomp, comps,  
    intercept = cumulative, se = FALSE, ...)

Arguments

object: an mvr object
estimate: a character vector. Which estimators to use. Should be a subset of c("all","train","CV","adjCV","test"). "adjCV" is only available for (R)MSEP. See below for how the estimators are chosen.
newdata: a data frame with test set data.
ncomp, comps: a vector of positive integers. The components or number of components to use. See below.
intercept: logical. Whether estimates for a model with zero components should be returned as well.
se: logical. Whether estimated standard errors of the estimates should be calculated. Not implemented yet.
...: further arguments sent to underlying functions or (for RMSEP) to MSEP
Details

RMSEP simply calls MSEP and takes the square root of the estimates. It therefore accepts the same arguments as MSEP.

Several estimators can be used. "train" is the training or calibration data estimate, also called (R)MSEC. For R2, this is the unadjusted $R^2$. It is overoptimistic and should not be used for assessing models. "CV" is the cross-validation estimate, and "adjCV" (for RMSEP and MSEP) is the bias-corrected cross-validation estimate. They can only be calculated if the model has been cross-validated. Finally, "test" is the test set estimate, using newdata as test set.

Which estimators to use is decided as follows (see below for mvrValstats). If estimate is not specified, the test set estimate is returned if newdata is specified, otherwise the CV and adjusted CV (for RMSEP and MSEP) estimates if the model has been cross-validated, otherwise the training data estimate. If estimate is "all", all possible estimates are calculated. Otherwise, the specified estimates are calculated.

Several model sizes can also be specified. If comps is missing (or is NULL), length(ncomp) models are used, with ncomp[1] components, ..., ncomp[length(ncomp)] components. Otherwise, a single model with the components comps[1], ..., comps[length(comps)] is used. If intercept is TRUE, a model with zero components is also used (in addition to the above).

The $R^2$ values returned by "R2" are calculated as $1 - SSE/SST$, where SST is the (corrected) total sum of squares of the response, and SSE is the sum of squared errors for either the fitted values (i.e., the residual sum of squares), test set predictions or cross-validated predictions (i.e., the PRESS). For estimate = "train", this is equivalent to the squared correlation between the fitted values and the response. For estimate = "train", the estimate is often called the prediction $R^2$.

mvrValstats is a utility function that calculates the statistics needed by MSEP and R2. It is not intended to be used interactively. It accepts the same arguments as MSEP and R2. However, the estimate argument must be specified explicitly: no partial matching and no automatic choice is made. The function simply calculates the types of estimates it knows, and leaves the other untouched.

Value

mvrValstats returns a list with components

- **SSE** three-dimensional array of SSE values. The first dimension is the different estimators, the second is the response variables and the third is the models.
- **SST** matrix of SST values. The first dimension is the different estimators and the second is the response variables.
- **nobj** a numeric vector giving the number of objects used for each estimator.
- **comps** the components specified, with 0 prepended if intercept is TRUE.
- **cumulative** TRUE if comps was NULL or not specified.

The other functions return an object of class "mvrVal", with components

- **val** three-dimensional array of estimates. The first dimension is the different estimators, the second is the response variables and the third is the models.
- **type** "MSEP", "RMSEP" or "R2".
- **comps** the components specified, with 0 prepended if intercept is TRUE.
**cumulative**  TRUE if `comps` was `NULL` or not specified.
**call**  the function call

**Author(s)**
Ron Wehrens and Bjørn-Helge Mevik

**References**

**See Also**
mvr, crossval, mvrCv, validationplot, plot.mvrVal

**Examples**
```r
data(oliveoil)
mod <- plsr(sensory ~ chemical, ncomp = 4, data = oliveoil, validation = "LOO")
RMSEP(mod)
## Not run: plot(R2(mod))
```

---

**oliveoil**  
*Sensory and physico-chemical data of olive oils*

---

**Description**
A data set with scores on 6 attributes from a sensory panel and measurements of 5 physico-chemical quality parameters on 16 olive oil samples. The first five oils are Greek, the next five are Italian and the last six are Spanish.

**Usage**
oliveoil

**Format**
A data frame with 16 observations on the following 2 variables.
chemical  a matrix with 5 columns. Measurements of acidity, peroxide, K232, K270, and DK.

**Source**
oscorespls.fit  Orthogonal scores PLSR

Description

Fits a PLSR model with the orthogonal scores algorithm (aka the NIPALS algorithm).

Usage

oscorespls.fit(X, Y, ncomp, center = TRUE, stripped = FALSE, 
                 tol = .Machine$double.eps^0.5, maxit = 100, ...)  

Arguments

X  a matrix of observations. NAs and Infs are not allowed.
Y  a vector or matrix of responses. NAs and Infs are not allowed.
ncomp  the number of components to be used in the modelling.
center  logical, determines if the X and Y matrices are mean centered or not. Default is to perform mean centering.
stripped  logical. If TRUE the calculations are stripped as much as possible for speed; this is meant for use with cross-validation or simulations when only the coefficients are needed. Defaults to FALSE.
tol  numeric. The tolerance used for determining convergence in multi-response models.
maxit  positive integer. The maximal number of iterations used in the internal Eigen-vector calculation.
...  other arguments. Currently ignored.

Details

This function should not be called directly, but through the generic functions plsr or mvr with the argument method="oscorespls". It implements the orthogonal scores algorithm, as described in Martens and Næs (1989). This is one of the two “classical” PLSR algorithms, the other being the orthogonal loadings algorithm.

Value

A list containing the following components is returned:

coefficients  an array of regression coefficients for 1, ..., ncomp components. The dimensions of coefficients are c(nvar, npred, ncomp) with nvar the number of X variables and npred the number of variables to be predicted in Y.
scores  a matrix of scores.
loadings  a matrix of loadings.
plot.mvr

loading.weights
a matrix of loading weights.
Yscores     a matrix of Y-scores.
Yloadings   a matrix of Y-loadings.
projection  the projection matrix used to convert X to scores.
Xmeans      a vector of means of the X variables.
Ymeans      a vector of means of the Y variables.
fitted.values an array of fitted values. The dimensions of fitted.values are c(nobj,npred,ncomp) with nobj the number samples and npred the number of Y variables.
residuals   an array of regression residuals. It has the same dimensions as fitted.values.
Xvar        a vector with the amount of X-variance explained by each component.
Xtotvar     Total variance in X.

If stripped is TRUE, only the components coefficients, Xmeans and Ymeans are returned.

Author(s)
Ron Wehrens and Bjørn-Helge Mevik

References

See Also
mvr plsr pcr kernelpls.fit widekernelpls.fit simpls.fit

Description
plot.mvr plots predictions, coefficients, scores, loadings, biplots, correlation loadings or validation plots (RMSEP curves, etc.).

Usage
## S3 method for class 'mvr'
plot(x, plottype = c("prediction", "validation", "coefficients",
                   "scores", "loadings", "biplot", "correlation"), ...)

Arguments
x          an object of class mvr. The fitted model to plot.
plottype   character. What kind of plot to plot.
...        further arguments, sent to the underlying plot functions.
Details

The function is simply a wrapper for the underlying plot functions used to make the selected plots. See `predplot.mvr`, `validationplot`, `coefplot`, `scoreplot`, `loadingplot`, `biplot.mvr` or `corrplot` for details. Note that all arguments except `x` and `plottype` must be named.

Value

`plot.mvr` returns whatever the underlying plot function returns.

Author(s)

Ron Wehrens and Bjørn-Helge Mevik

See Also

`mvr`, `predplot.mvr`, `validationplot`, `coefplot`, `scoreplot`, `loadingplot`, `biplot.mvr`, `corrplot`

Examples

data(yarn)
nir.pcr <- pcr(density ~ NIR, ncomp = 9, data = yarn, validation = "CV")
## Not run:
plot(nir.pcr, ncomp = 5) # Plot of cross-validated predictions
plot(nir.pcr, "scores") # Score plot
plot(nir.pcr, "loadings", comps = 1:3) # The three first loadings
plot(nir.pcr, "coef", ncomp = 5) # Coefficients
plot(nir.pcr, "val") # RMSEP curves
plot(nir.pcr, "val", val.type = "MSEP", estimate = "CV") # CV MSEP
## End(Not run)

pls.options

Set or return options for the pls package

Description

A function to set options for the `pls` package, or to return the current options.

Usage

`pls.options(...)`

Arguments

... a single list, a single character vector, or any number of named arguments (`name = value`).
If called with no arguments, or with an empty list as the single argument, `pls.options` returns the current options.

If called with a character vector as the single argument, a list with the arguments named in the vector are returned.

If called with a non-empty list as the single argument, the list elements should be named, and are treated as named arguments to the function.

Otherwise, `pls.options` should be called with one or more named arguments `name = value`. For each argument, the option named `name` will be given the value `value`.

The recognised options are:

- `mvralg`: The fit method to use in `mvr` and `mvrCv`. The value should be one of the allowed methods. Defaults to "kernelpls". Can be overridden with the argument method in `mvr` and `mvrCv`.

- `pcralg`: The fit method to use in `pcr`. The value should be one of the allowed methods. Defaults to "svdpc". Can be overridden with the argument method in `pcr`.

- `plsralg`: The fit method to use in `plsr`. The value should be one of the allowed methods. Defaults to "kernelpls". Can be overridden with the argument method in `plsr`.

- `cpplsalg`: The fit method to use in `cppls`. The value should be one of the allowed methods. Defaults to "cppls". Can be overridden with the argument method in `cppls`.

- `parallel`: Specification of how the cross-validation (CV) in `mvr` should be performed. If the specification is `NULL` (default) or 1, the CV is done serially, otherwise it is done in parallel using functionality from the `parallel` package.

- `w.tol`: The tolerance used for removing values close to 0 in the vectors of loading weights in `cppls`. Defaults to `.Machine$double.eps`.

- `X.tol`: The tolerance used for removing predictor variables with L1 norms close to 0 in `cppls`. Defaults to $10^{-12}$.

The function is a slight modification of the function `sm.options` from the package `sm`. 
**predict.mvr**

*Predict Method for PLSR and PCR*

**Description**

Prediction for mvr (PCR, PLSR) models. New responses or scores are predicted using a fitted model and a new matrix of observations.

**Usage**

```r
## S3 method for class 'mvr'
predict(object, newdata, ncomp = 1:object$ncomp, comps, 
        type = c("response", "scores"), na.action = na.pass, ...)
```

**Arguments**

- **object**: an mvr object. The fitted model
- **newdata**: a data frame. The new data. If missing, the training data is used.
- **ncomp, comps**: vector of positive integers. The components to use in the prediction. See below.
- **type**: character. Whether to predict scores or response values
- **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
Details

When type is "response" (default), predicted response values are returned. If comps is missing (or is NULL), predictions for length(ncomp) models with ncomp[1] components, ncomp[2] components, etc., are returned. Otherwise, predictions for a single model with the exact components in comps are returned. (Note that in both cases, the intercept is always included in the predictions. It can be removed by subtracting the Ymeans component of the fitted model.)

When type is "scores", predicted score values are returned for the components given in comps. If comps is missing or NULL, ncomps is used instead.

It is also possible to supply a matrix instead of a data frame as newdata, which is then assumed to be the X data matrix. Note that the usual checks for the type of the data are then omitted. Also note that this is only possible with predict; it will not work in functions like predplot, RMSEP or R2, because they also need the response variable of the new data.

Value

When type is "response", a three dimensional array of predicted response values is returned. The dimensions correspond to the observations, the response variables and the model sizes, respectively. When type is "scores", a score matrix is returned.

Note

A warning message like ‘newdata’ had 10 rows but variable(s) found have 106 rows’ means that not all variables were found in the newdata data frame. This (usually) happens if the formula contains terms like yarn$NIR. Do not use such terms; use the data argument instead. See mvr for details.

Author(s)

Ron Wehrens and Bjørn-Helge Mevik

See Also

mvr, summary.mvr, coef.mvr, plot.mvr

Examples

data(yarn)
nir.mvr <- mvr(density ~ NIR, ncomp = 5, data = yarn[yarn$train,])

## Predicted responses for models with 1, 2, 3 and 4 components
pred.resp <- predict(nir.mvr, ncomp = 1:4, newdata = yarn[!yarn$train,])

## Predicted responses for a single model with components 1, 2, 3, 4
predict(nir.mvr, comps = 1:4, newdata = yarn[!yarn$train,])

## Predicted scores
predict(nir.mvr, comps = 1:3, type = "scores", newdata = yarn[!yarn$train,])
Description

Functions to plot predicted values against measured values for a fitted model.

Usage

predplot(object, ...)  
## Default S3 method:  
predplot(object, ...)  
## S3 method for class 'mvr'  
predplot(object, ncomp = object$ncomp, which, newdata, nCols,  
nRows, xlab = "measured", ylab = "predicted", main,  
ask = nRows * nCols < nPlots && dev.interactive(),  
..., font.main, cex.main)

predplotXy(x, y, line = FALSE, labels, type = "p", main = "Prediction plot",  
xlab = "measured response", ylab = "predicted response",  
line.col = par("col"), line.lty = NULL, line.lwd = NULL, ...)

Arguments

object  
a fitted model.

ncomp  
integer vector. The model sizes (numbers of components) to use for prediction.

which  
character vector. Which types of predictions to plot. Should be a subset of  
c("train","validation","test"). If not specified, plot.mvr selects test set  
predictions if newdata is supplied, otherwise cross-validated predictions if the  
model has been cross-validated, otherwise fitted values from the calibration data.

newdata  
data frame. New data to predict.

nCols, nRows  
integer. The number of columns and rows the plots will be laid out in. If not  
specified, plot.mvr tries to be intelligent.

xlab, ylab  
titles for x and y axes. Typically character strings, but can be expressions or  
lists. See title for details.

labels  
optional. Alternative plot labels to use. Either a vector of labels, or "names" or  
"numbers" to use the row names or row numbers of the data as labels.

type  
character. What type of plot to make. Defaults to "p" (points). See plot for a  
complete list of types. The argument is ignored if labels is specified.

main  
optional main title for the plot. See Details.

ask  
logical. Whether to ask the user before each page of a plot.

font.main  
font to use for main titles. See par for details. Also see Details below.

cex.main  
numeric. The magnification to be used for main titles relative to the current size.  
Also see Details below.
predplot

x numeric vector. The observed response values.
y numeric vector. The predicted response values.
line logical. Whether a target line should be drawn.
line.col, line.lty, line.lwd character or numeric. The col, lty and lwd parameters for the target line. See par for details.
... further arguments sent to underlying plot functions.

Details

predplot is a generic function for plotting predicted versus measured response values, with default and mvr methods currently implemented. The default method is very simple, and doesn’t handle multiple responses or new data.

The mvr method, handles multiple responses, model sizes and types of predictions by making one plot for each combination. It can also be called through the plot method for mvr, by specifying plottype = "prediction" (the default).

The argument main can be used to specify the main title of the plot. It is handled in a non-standard way. If there is only on (sub) plot, main will be used as the main title of the plot. If there is more than one (sub) plot, however, the presence of main will produce a corresponding ‘global’ title on the page. Any graphical parameters, e.g., cex.main, supplied to coefplot will only affect the ‘ordinary’ plot titles, not the ‘global’ one. Its appearance can be changed by setting the parameters with par, which will affect both titles (with the exception of font.main and cex.main, which will only affect the ‘global’ title when there is more than one plot). (To have different settings for the two titles, one can override the par settings with arguments to predplot.)

cpredplotXY is an internal function and is not meant for interactive use. It is called by the predplot methods, and its arguments, e.g, line, can be given in the predplot call.

Value

The functions invisibly return a matrix with the (last) plotted data.

Note

The font.main and cex.main must be (completely) named. This is to avoid that any argument cex or font matches them.

Tip: If the labels specified with labels are too long, they get clipped at the border of the plot region. This can be avoided by supplying the graphical parameter xpd = TRUE in the plot call.

Author(s)

Ron Wehrens and Bjørn-Helge Mevik

See Also

mvr, plot.mvr
Examples

data(yarn)
mod <- pls(r(density ~ NIR, ncomp = 10, data = yarn[train,], validation = "CV")
## Not run:
predplot(mod, ncomp = 1:6)
plot(mod, ncomp = 1:6) # Equivalent to the previous
## Both cross-validated and test set predictions:
predplot(mod, ncomp = 4:6, which = c("validation", "test"),
    newdata = yarn[!train,])
## End(Not run)

data(oliveoil)
mod.sens <- pls(sensory ~ chemical, ncomp = 4, data = oliveoil)
## Not run: plot(mod.sens, ncomp = 2:4) # Several responses gives several plots

scoreplot

Plots of Scores, Loadings and Correlation Loadings

Description

Functions to make scatter plots of scores or correlation loadings, and scatter or line plots of loadings.

Usage

scoreplot(object, ...)
## Default S3 method:
scoreplot(object, comps = 1:2, labels, identify = FALSE, type = "p",
    xlab, ylab, ...)  
## S3 method for class 'scores'
plot(x, ...)

loadingplot(object, ...)
## Default S3 method:
loadingplot(object, comps = 1:2, scatter = FALSE, labels,
    identify = FALSE, type, lty, lwd = NULL, pch, cex = NULL,
    col, legendpos, xlab, ylab, pretty.xlabels = TRUE, xlim, ...)  
## S3 method for class 'loadings'
plot(x, ...)

corrplot(object, comps = 1:2, labels, plotx = TRUE, ploty = FALSE,
    radii = c(sqrt(1/2), 1), identify = FALSE, type = "p",
    xlab, ylab, col, ...)

Arguments

object  an R object. The fitted model.
comps       integer vector. The components to plot.
scatter  logical. Whether the loadings should be plotted as a scatter instead of as lines.
labels  optional. Alternative plot labels or x axis labels. See Details.
plotx  logical. Whether to plot the X correlation loadings. Defaults to TRUE.
ploty  logical. Whether to plot the Y correlation loadings. Defaults to FALSE.
radii  numeric vector, giving the radii of the circles drawn in corrplot. The default radii represent 50% and 100% explained variance of the X variables by the chosen components.
identify  logical. Whether to use identify to interactively identify points. See below.
type  character. What type of plot to make. Defaults to "p" (points) for scatter plots and "l" (lines) for line plots. See plot for a complete list of types (not all types are possible/meaningful for all plots).
lty  vector of line types (recycled as necessary). Line types can be specified as integers or character strings (see par for the details).
lwd  vector of positive numbers (recycled as necessary), giving the width of the lines.
pch  plot character. A character string or a vector of single characters or integers (recycled as necessary). See points for all alternatives.
cex  numeric vector of character expansion sizes (recycled as necessary) for the plotted symbols.
col  character or integer vector of colors for plotted lines and symbols (recycled as necessary). See par for the details.
legendpos  Legend position. Optional. Ignored if scatter is TRUE. If present, a legend is drawn at the given position. The position can be specified symbolically (e.g., legendpos = "topright"). This requires R >= 2.1.0. Alternatively, the position can be specified explicitly (legendpos = t(c(x,y))) or interactively (legendpos = locator()).
xlab,ylab  titles for x and y axes. Typically character strings, but can be expressions or lists. See title for details.
pretty.xlabels  logical. If TRUE, loadingplot tries to plot the x labels more nicely. See Details.
xlim  optional vector of length two, with the x limits of the plot.
x  a scores or loadings object. The scores or loadings to plot.
...  further arguments sent to the underlying plot function(s).

Details

plot.scores is simply a wrapper calling scoreplot, passing all arguments. Similarly for plot.loadings.

scoreplot is generic, currently with a default method that works for matrices and any object for which scores returns a matrix. The default scoreplot method makes one or more scatter plots of the scores, depending on how many components are selected. If one or two components are selected, and identify is TRUE, the function identify is used to interactively identify points.

Also loadingplot is generic, with a default method that works for matrices and any object where loadings returns a matrix. If scatter is TRUE, the default method works exactly like the default scoreplot method. Otherwise, it makes a lineplot of the selected loading vectors, and if identify
is TRUE, uses **identify** to interactively identify points. Also, if `legendpos` is given, a legend is drawn at the position indicated.

corrplot works exactly like the default scoreplot method, except that at least two components must be selected. The “correlation loadings”, i.e. the correlations between each variable and the selected components (see References), are plotted as pairwise scatter plots, with concentric circles of radii given by `radii`. Each point corresponds to a variable. The squared distance between the point and origin equals the fraction of the variance of the variable explained by the components in the panel. The default `radii` corresponds to 50% and 100% explained variance. By default, only the correlation loadings of the \( X \) variables are plotted, but if `ploty` is TRUE, also the \( Y \) correlation loadings are plotted.

scoreplot, loadingplot and corrplot can also be called through the plot method for mvr objects, by specifying plottype as "scores", "loadings" or "correlation", respectively. See `plot.mvr`.

The argument `labels` can be a vector of labels or one of "names" and "numbers".

If a scatter plot is produced (i.e., scoreplot, corrplot, or loadingplot with scatter = TRUE), the labels are used instead of plot symbols for the points plotted. If labels is "names" or "numbers", the row names or row numbers of the matrix (scores, loadings or correlation loadings) are used.

If a line plot is produced (i.e., loadingplot), the labels are used as \( x \) axis labels. If labels is "names" or "numbers", the variable names are used as labels, the difference being that with "numbers", the variable names are converted to numbers, if possible. Variable names of the forms "'number'" or "'number text'" (where the space is optional), are handled.

The argument `pretty.xlabels` is only used when `labels` is specified for a line plot. If TRUE (default), the code tries to use a ‘pretty’ selection of labels. If labels is "numbers", it also uses the numerical values of the labels for horizontal spacing. If one has excluded parts of the spectral region, one might therefore want to use `pretty.xlabels = FALSE`.

**Value**

The functions return whatever the underlying plot function (or **identify**) returns.

**Note**

`legend` has many options. If you want greater control over the appearance of the legend, omit the `legendpos` argument and call **legend** manually.

Graphical parameters (such as `pch` and `cex`) can also be used with scoreplot and corrplot. They are not listed in the argument list simply because they are not handled specifically in the function (unlike in loadingplot), but passed directly to the underlying plot functions by ....

Tip: If the labels specified with `labels` are too long, they get clipped at the border of the plot region. This can be avoided by supplying the graphical parameter `xpd = TRUE` in the plot call.

The handling of `labels` and `pretty.xlabels` in coefplot is experimental.

**Author(s)**

Ron Wehrens and Bjørn-Helge Mevik
Scores

References


See Also

mvr, plot.mvr, scores, loadings, identify, legend

Examples

data(yarn)
mod <- plsr(density ~ NIR, ncomp = 10, data = yarn)
## These three are equivalent:
## Not run:
scoreplot(mod, comps = 1:5)
plot(scores(mod), comps = 1:5)
plot(mod, plottype = "scores", comps = 1:5)

loadingplot(mod, comps = 1:5)
loadingplot(mod, comps = 1:5, legendpos = "topright") # With legend
loadingplot(mod, comps = 1:5, scatter = TRUE) # Plot as scatterplots

corrplot(mod, comps = 1:2)
corrplot(mod, comps = 1:3)

## End(Not run)

scores

Extract Scores and Loadings from PLSR and PCR Models

Description

These functions extract score and loading matrices from fitted mvr models.

Usage

scores(object, ...)
## Default S3 method:
scores(object, ...)

loadings(object, ...)
## Default S3 method:
loadings(object, ...)

loading.weights(object)

Yscores(object)

Yloadings(object)
selectNcomp

Arguments

object a fitted model to extract from.
... extra arguments, currently not used.

Details

All functions extract the indicated matrix from the fitted model, and will work with any object having a suitably named component.

The default scores and loadings methods also handle prcomp objects (their scores and loadings components are called x and rotation, resp.), and add an attribute "explvar" with the variance explained by each component, if this is available. (See explvar for details.)

Value

A matrix with scores or loadings.

Note

There is a loadings function in package stats. It simply returns any element named "loadings". See loadings for details. The function can be accessed as stats::loadings(...).

Author(s)

Ron Wehrens and Bjørn-Helge Mevik

See Also

mvr, coef.mvr

Examples

data(yarn)
plsmod <- plsr(density ~ NIR, 6, data = yarn)
scores(plsmod)
loadings(plsmod)[,1:4]

suggestNcomp

Suggestions for the optimal number of components in PCR and PLSR models

Description

Choosing the best number of components in PCR and PLSR models is difficult and usually done on the basis of visual inspection of the validation plots. In cases where large numbers of models are built this choice needs to be automated. This function implements two proposals, one based on randomization (permutation) testing, and an approach based on the standard error of the cross-validation residuals.
selectNcomp

Usage

selectNcomp(object, method = c("randomization", "onesigma"),
            nperm = 999, alpha = 0.01, ncomp = object$ncomp,
            plot = FALSE, ...)

Arguments

object an mvr object. The fitted model. It should contain a validation element.
method character string, indicating the heuristic to use.
nperm number of permutations in the "randomization" approach - not used in the "onesigma" approach.
alpha cutoff for p values in the "randomization" approach - not used in the "onesigma" approach.
ncomp maximum number of components to consider when determining the global minimum in the cross-validation curve.
plot whether or not to show a cross-validation plot. The plot for the "randomization" approach shows models that do not differ significantly from the global RMSEP minimum with open circles; the "onesigma" approach shows the one-sigma bands around the RMSEP values. In both cases, the selection is indicated with a blue dashed line.
...
Further plotting arguments, e.g., to add a title to the plot, or to limit the plotting range.

Details

In both approaches the results of cross-validation are used, so the model should have been calculated with some form of cross-validation. First, the absolute minimum in the CV curve is determined (considering only the first ncomp components), leading to the reference model. The randomization test approach (Van der Voet, 1994) checks whether the squared prediction errors of models with fewer components are significantly larger than in the reference model. This leads for each model considered to a p value; the smallest model not significantly worse than the reference model is returned as the selected one.

The approach "onesigma" simply returns the first model where the optimal CV is within one standard error of the absolute optimum (Hastie, Tibshirani and Friedman, 2009). Note that here we simply use the standard deviation of the cross-validation residuals, in line with the procedure used to calculate the error measure itself. Some other packages implementing similar procedures (such as glmnet) calculate an error measure for each validation segment separately and use the average as the final estimate. In such cases the standard error across segments is the relevant measure of spread. For LOO, the two procedures are identical. In other forms of validation, small differences will occur.

Value

A number indicating the suggested number of components in the model.
**simpls.fit**

**Sijmen de Jong’s SIMPLS**

Fits a PLSR model with the SIMPLS algorithm.

**Usage**

`simpls.fit(X, Y, ncomp, center = TRUE, stripped = FALSE, ...)`

**Arguments**

- **X**
  - a matrix of observations. NAs and Infs are not allowed.
- **Y**
  - a vector or matrix of responses. NAs and Infs are not allowed.
- **ncomp**
  - the number of components to be used in the modelling.
- **center**
  - logical, determines if the X and Y matrices are mean centered or not. Default is to perform mean centering.
- **stripped**
  - logical. If TRUE the calculations are stripped as much as possible for speed; this is meant for use with cross-validation or simulations when only the coefficients are needed. Defaults to FALSE.
- **...**
  - other arguments. Currently ignored.

**Description**

Fits a PLSR model with the SIMPLS algorithm.

**References**


**See Also**

- `mvr`, `summary.mvr`

**Examples**

```r
data(yarn)
yarn.pls <- plsr(density ~ NIR, data = yarn, scale = TRUE, ncomp = 20, validation = "LOO")
selectNcomp(yarn.pls, "onesigma", plot = TRUE, ylim = c(0, 3))
selectNcomp(yarn.pls, "randomization", plot = TRUE)
selectNcomp(yarn.pls, "randomization", plot = TRUE, ncomp = 10, ylim = c(0, 3))
```
Details

This function should not be called directly, but through the generic functions `plsr` or `mvr` with the argument `method="simpls"`. SIMPLS is much faster than the NIPALS algorithm, especially when the number of X variables increases, but gives slightly different results in the case of multivariate Y. SIMPLS truly maximises the covariance criterion. According to de Jong, the standard PLS2 algorithms lie closer to ordinary least-squares regression where a precise fit is sought; SIMPLS lies closer to PCR with stable predictions.

Value

A list containing the following components is returned:

- `coefficients`: an array of regression coefficients for 1, ..., ncomp components. The dimensions of coefficients are `c(nvar,npred,ncomp)` with `nvar` the number of X variables and `npred` the number of variables to be predicted in Y.
- `scores`: a matrix of scores.
- `loadings`: a matrix of loadings.
- `projection`: the projection matrix used to convert X to scores.
- `Xmeans`: a vector of means of the X variables.
- `Ymeans`: a vector of means of the Y variables.
- `fitted.values`: an array of fitted values. The dimensions of fitted.values are `c(nobj,npred,ncomp)` with `nobj` the number samples and `npred` the number of Y variables.
- `residuals`: an array of regression residuals. It has the same dimensions as fitted.values.
- `Xvar`: a vector with the amount of X-variance explained by each component.
- `Xtotvar`: Total variance in X.

If stripped is TRUE, only the components coefficients, Xmeans and Ymeans are returned.

Author(s)

Ron Wehrens and Bjørn-Helge Mevik

References


See Also

`mvr`, `plsr`, `pcr`, `kernelpls.fit`, `widekernelpls.fit`, `oscorespls.fit`
**stdize**  
*Standardization of Data Matrices*

**Description**
Performs standardization (centering and scaling) of a data matrix.

**Usage**

```r
stdize(x, center = TRUE, scale = TRUE)
```

## S3 method for class 'stdize'

```r
predict(object, newdata, ...)
```

## S3 method for class 'stdize'

```r
makepredictcall(var, call)
```

**Arguments**

- `x, newdata`  
  numeric matrices. The data to standardize.
- `center`  
  logical value or numeric vector of length equal to the number of columns of `x`.
- `scale`  
  logical value or numeric vector of length equal to the number of columns of `x`.
- `object`  
  an object inheriting from class "stdize", normally the result of a call to `stdize`.
- `var`  
  A variable.
- `call`  
  The term in the formula, as a call.
- `...`  
  other arguments. Currently ignored.

**Details**

`makepredictcall.stdized` is an internal utility function; it is not meant for interactive use. See `makepredictcall` for details.

If `center` is `TRUE`, `x` is centered by subtracting the column mean from each column. If `center` is a numeric vector, it is used in place of the column means.

If `scale` is `TRUE`, `x` is scaled by dividing each column by its sample standard deviation. If `scale` is a numeric vector, it is used in place of the standard deviations.

**Value**

Both `stdize` and `predict.stdize` return a scaled and/or centered matrix, with attributes "stdize:center" and/or "stdize:scale" the vector used for centering and/or scaling. The matrix is given class c("stdize","matrix").

**Note**

`stdize` is very similar to `scale`. The difference is that when `scale = TRUE`, `stdize` divides the columns by their standard deviation, while `scale` uses the root-mean-square of the columns. If `center` is `TRUE`, this is equivalent, but in general it is not.
Author(s)
Bjørn-Helge Mevik and Ron Wehrens

See Also
mvr, pcr, plsr, msc, scale

Examples

data(yarn)
## Direct standardization:
Ztrain <- stdize(yarn$NIR[yarn$train,])
Ztest <- predict(Ztrain, yarn$NIR[!yarn$train,])

## Used in formula:
mod <- plsr(density ~ stdize(NIR), ncomp = 6, data = yarn[yarn$train,])
pred <- predict(mod, newdata = yarn[!yarn$train,]) # Automatically standardized

---

summary.mvr

Summary and Print Methods for PLSR and PCR objects

Description
Summary and print methods for mvr and mvrVal objects.

Usage
## S3 method for class 'mvr'
summary(object, what = c("all", "validation", "training"),
digits = 4, print.gap = 2, ...)
## S3 method for class 'mvr'
print(x, ...)
## S3 method for class 'mvrVal'
print(x, digits = 4, print.gap = 2, ...)

Arguments
x, object an mvr object
what one of "all", "validation" or "training"
digits integer. Minimum number of significant digits in the output. Default is 4.
print.gap Integer. Gap between columns of the printed tables.
... Other arguments sent to underlying methods.

details
If what is "training", the explained variances are given; if it is "validation", the cross-validated
RMSEPs (if available) are given; if it is "all", both are given.
svdpc.fit

Value

print.mvr and print.mvrVal return the object invisibly.

Author(s)

Ron Wehrens and Bjørn-Helge Mevik

See Also

mvr, pcr, plsr, RMSEP, MSEP

Examples

data(yarn)
nir.mvr <- mvr(density ~ NIR, ncomp = 8, validation = "LOO", data = yarn)
nir.mvr
summary(nir.mvr)
RMSEP(nir.mvr)

svdpc.fit Principal Component Regression

Description

Fits a PCR model using the singular value decomposition.

Usage

svdpc.fit(X, Y, ncomp, center = TRUE, stripped = FALSE, ...)

Arguments

X

a matrix of observations. NAs and Infs are not allowed.

Y

a vector or matrix of responses. NAs and Infs are not allowed.

ncomp

the number of components to be used in the modelling.

center

logical, determines if the X and Y matrices are mean centered or not. Default is to perform mean centering.

stripped

logical. If TRUE the calculations are stripped as much as possible for speed; this is meant for use with cross-validation or simulations when only the coefficients are needed. Defaults to FALSE.

...

other arguments. Currently ignored.

Details

This function should not be called directly, but through the generic functions pcr or mvr with the argument method="svdpc". The singular value decomposition is used to calculate the principal components.
Value

A list containing the following components is returned:

- **coefficients**: an array of regression coefficients for 1,..., ncomp components. The dimensions of coefficients are c(nvar, npred, ncomp) with nvar the number of X variables and npred the number of variables to be predicted in Y.
- **scores**: a matrix of scores.
- **loadings**: a matrix of loadings.
- **Yloadings**: a matrix of Y-loadings.
- **projection**: the projection matrix used to convert X to scores.
- **Xmeans**: a vector of means of the X variables.
- **Ymeans**: a vector of means of the Y variables.
- **fitted.values**: an array of fitted values. The dimensions of fitted.values are c(nobj, npred, ncomp) with nobj the number samples and npred the number of Y variables.
- **residuals**: an array of regression residuals. It has the same dimensions as fitted.values.
- **Xvar**: a vector with the amount of X-variance explained by each component.
- **Xtotvar**: Total variance in X.

If stripped is TRUE, only the components coefficients, Xmeans and Ymeans are returned.

Author(s)

Ron Wehrens and Bjørn-Helge Mevik

References


See Also

- mvr
- plsr
- pcr
- cppls

Description

Functions to plot validation statistics, such as RMSEP or $R^2$, as a function of the number of components.
validationplot

Usage

validationplot(object, val.type = c("RMSEP", "MSEP", "R2"), estimate,
               newdata, ncomp, comps, intercept, ...)

## S3 method for class 'mvrVal'
plot(x, nCols, nRows, type = "l", lty = 1:nEst,
     lwd = par("lwd"), pch = 1:nEst, cex = 1, col = 1:nEst, legendpos,
     xlab = "number of components", ylab = x$type, main,
     ask = nRows * nCols < nResp && dev.interactive(), ...)

Arguments

object an mvr object.
val.type character. What type of validation statistic to plot.
estimate character. Which estimates of the statistic to calculate. See RMSEP.
newdata data frame. Optional new data used to calculate statistic.
ncomp, comps integer vector. The model sizes to compute the statistic for. See RMSEP.
intercept logical. Whether estimates for a model with zero components should be calculated as well.
x an mvrVal object. Usually the result of a RMSEP, MSEP or R2 call.
nCols, nRows integers. The number of columns and rows the plots will be laid out in. If not specified, plot.mvrVal tries to be intelligent.
type character. What type of plots to create. Defaults to "l" (lines). Alternative types include "p" (points) and "b" (both). See plot for a complete list of types.
lty vector of line types (recycled as necessary). Line types can be specified as integers or character strings (see par for the details).
lwd vector of positive numbers (recycled as necessary), giving the width of the lines.
pch plot character. A character string or a vector of single characters or integers (recycled as necessary). See points for all alternatives.
cex numeric vector of character expansion sizes (recycled as necessary) for the plotted symbols.
col character or integer vector of colors for plotted lines and symbols (recycled as necessary). See par for the details.
legendpos Legend position. Optional. If present, a legend is drawn at the given position.
   The position can be specified symbolically (e.g., legendpos = "topleft"). This requires R >= 2.1.0. Alternatively, the position can be specified explicitly (legendpos = t(c(x,y))) or interactively (legendpos = locator()). This only works well for plots of single-response models.
xlab, ylab titles for x and y axes. Typically character strings, but can be expressions (e.g., expression(R^2) or lists. See title for details.
main optional main title for the plot. See Details.
ask logical. Whether to ask the user before each page of a plot.
... Further arguments sent to underlying plot functions.
validationplot calls the proper validation function (currently \texttt{MSEP}, \texttt{RMSEP} or \texttt{R2}) and plots the results with \texttt{plot.mvrVal}. validationplot can be called through the \texttt{mvr plot} method, by specifying \texttt{plottype = "validation"}.

\texttt{plot.mvrVal} creates one plot for each response variable in the model, laid out in a rectangle. It uses \texttt{matplot} for performing the actual plotting. If \texttt{legendpos} is given, a legend is drawn at the given position.

The argument \texttt{main} can be used to specify the main title of the plot. It is handled in a non-standard way. If there is only on (sub) plot, \texttt{main} will be used as the main title of the plot. If there is more than one (sub) plot, however, the presence of \texttt{main} will produce a corresponding ‘global’ title on the page. Any graphical parameters, e.g., \texttt{cex.main}, supplied to \texttt{coefplot} will only affect the ‘ordinary’ plot titles, not the ‘global’ one. Its appearance can be changed by setting the parameters with \texttt{par}, which will affect both titles. (To have different settings for the two titles, one can override the \texttt{par} settings with arguments to the plot function.)

\textbf{Note}

\texttt{legend} has many options. If you want greater control over the appearance of the legend, omit the \texttt{legendpos} argument and call \texttt{legend} manually.

\textbf{Author(s)}

Ron Wehrens and Bjørn-Helge Mevik

\textbf{See Also}

\texttt{mvr, plot.mvr, RMSEP, MSEP, R2, matplot, legend}

\textbf{Examples}

```r
data(oliveoil)
mod <- plsrt(sensory ~ chemical, data = oliveoil, validation = "LOO")
## Not run:
## These three are equivalent:
validationplot(mod, estimate = "all")
plot(mod, "validation", estimate = "all")
plot(RMSEP(mod, estimate = "all"))
## Plot R2:
plot(mod, "validation", val.type = "R2")
## Plot R2, with a legend:
plot(mod, "validation", val.type = "MSEP", legendpos = "top") # R >= 2.1.0
```

## End(Not run)
**Description**

Calculates jackknife variance or covariance estimates of regression coefficients.

**Usage**

`var.jack(object, ncomp = object$ncomp, covariance = FALSE, use.mean = TRUE)`

**Arguments**

- **object**: an `mvr` object. A cross-validated model fitted with `jackknife = TRUE`.
- **ncomp**: the number of components to use for estimating the (co)variances.
- **covariance**: logical. If `TRUE`, covariances are calculated; otherwise only variances. The default is `FALSE`.
- **use.mean**: logical. If `TRUE` (default), the mean coefficients are used when estimating the (co)variances; otherwise the coefficients from a model fitted to the entire data set. See Details.

**Details**

The original (Tukey) jackknife variance estimator is defined as $(g-1)/g \sum_{i=1}^{g} (\tilde{\beta}_{-i} - \bar{\beta})^2$, where $g$ is the number of segments, $\tilde{\beta}_{-i}$ is the estimated coefficient when segment $i$ is left out (called the jackknife replicates), and $\bar{\beta}$ is the mean of the $\tilde{\beta}_{-i}$. The most common case is delete-one jackknife, with $g = n$, the number of observations.

This is the definition `var.jack` uses by default.

However, Martens and Martens (2000) defined the estimator as $(g-1)/g \sum_{i=1}^{g} (\hat{\beta}_{-i} - \hat{\beta})^2$, where $\hat{\beta}$ is the coefficient estimate using the entire data set. I.e., they use the original fitted coefficients instead of the mean of the jackknife replicates. Most (all?) other jackknife implementations for PLSR use this estimator. `var.jack` can be made to use this definition with `use.mean = FALSE`. In practice, the difference should be small if the number of observations is sufficiently large. Note, however, that all theoretical results about the jackknife refer to the ‘proper’ definition. (Also note that this option might disappear in a future version.)

**Value**

If `covariance` is `FALSE`, an $p \times q \times c$ array of variance estimates, where $p$ is the number of predictors, $q$ is the number of responses, and $c$ is the number of components.

If `covariance` is `TRUE`, an $pq \times pq \times c$ array of variance-covariance estimates.
Warning

Note that the Tukey jackknife variance estimator is not unbiased for the variance of regression coefficients (Hinkley 1977). The bias depends on the \( X \) matrix. For ordinary least squares regression (OLSR), the bias can be calculated, and depends on the number of observations \( n \) and the number of parameters \( k \) in the mode. For the common case of an orthogonal design matrix with \( \pm 1 \) levels, the delete-one jackknife estimate equals \( (n - 1)/(n - k) \) times the classical variance estimate for the regression coefficients in OLSR. Similar expressions hold for delete-\( d \) estimates. Modifications have been proposed to reduce or eliminate the bias for the OLSR case, however, they depend on the number of parameters used in the model. See e.g. Hinkley (1977) or Wu (1986).

Thus, the results of \texttt{var.jack} should be used with caution.

Author(s)

Bjørn-Helge Mevik

References


See Also

\texttt{mvrCv}, \texttt{jack.test}

Examples

```r
data(oliveoil)
mod <- pcr(sensory ~ chemical, data = oliveoil, validation = "LOO",
           jackknife = TRUE)
var.jack(mod, ncomp = 2)
```

widekernelpls.fit

Wide Kernel PLS (Rännar et al.)

Description

Fits a PLSR model with the wide kernel algorithm.
Usage

widekernelpls.fit(X, Y, ncomp, center = TRUE, stripped = FALSE,
    tol = .Machine$double.eps^0.5, maxit = 100, ...)

Arguments

X a matrix of observations. NAs and Infs are not allowed.
Y a vector or matrix of responses. NAs and Infs are not allowed.
ncomp the number of components to be used in the modelling.
center logical, determines if the X and Y matrices are mean centered or not. Default is to perform mean centering.
stripped logical. If TRUE the calculations are stripped as much as possible for speed; this is meant for use with cross-validation or simulations when only the coefficients are needed. Defaults to FALSE.
tol numeric. The tolerance used for determining convergence in the algorithm.
maxit positive integer. The maximal number of iterations used in the internal Eigen-vector calculation.
... other arguments. Currently ignored.

Details

This function should not be called directly, but through the generic functions plsr or mvr with the argument method="widekernelpls". The wide kernel PLS algorithm is efficient when the number of variables is (much) larger than the number of observations. For very wide X, for instance 12x18000, it can be twice as fast as kernelpls.fit and simpls.fit. For other matrices, however, it can be much slower. The results are equal to the results of the NIPALS algorithm.

Value

A list containing the following components is returned:

coefficients an array of regression coefficients for 1,..., ncomp components. The dimensions of coefficients are c(nvar,npred,ncomp) with nvar the number of X variables and npred the number of variables to be predicted in Y.
scores a matrix of scores.
loadings a matrix of loadings.
loading.weights a matrix of loading weights.
Yscores a matrix of Y-scores.
Yloadings a matrix of Y-loadings.
projection the projection matrix used to convert X to scores.
Xmeans a vector of means of the X variables.
Ymeans a vector of means of the Y variables.
fitted.values  an array of fitted values. The dimensions of fitted.values are c(nobj,npred,ncomp)
with nobj the number samples and npred the number of Y variables.
residuals  an array of regression residuals. It has the same dimensions as fitted.values.
Xvar  a vector with the amount of X-variance explained by each component.
Xtotvar  Total variance in X.

If stripped is TRUE, only the components coefficients, Xmeans and Ymeans are returned.

Note
The current implementation has not undergone extensive testing yet, and should perhaps be regarded
as experimental. Specifically, the internal Eigenvector calculation does not always converge in
extreme cases where the Eigenvalue is close to zero. However, when it does converge, it always
converges to the same results as kernelpls.fit, up to numerical inaccuracies.

The algorithm also has a bit of overhead, so when the number of observations is moderately high,
kernelpls.fit can be faster even if the number of predictors is much higher. The relative speed of
the algorithms can also depend greatly on which BLAS and/or LAPACK library R is linked against.

Author(s)
Bjørn-Helge Mevik

References
Many Variables and Fewer Objects. Part 1: Theory and Algorithm. Journal of Chemometrics, 8,
111–125.

See Also
mvr plsr cppls pcr kernelpls.fit simpls.fit oscorespls.fit

yarn  NIR spectra and density measurements of PET yarns

Description
A training set consisting of 21 NIR spectra of PET yarns, measured at 268 wavelengths, and 21
corresponding densities. A test set of 7 samples is also provided. Many thanks to Erik Swierenga.

Usage
yarn
yarn

Format

A data frame with components

- **NIR**  Numeric matrix of NIR measurements
- **density**  Numeric vector of densities
- **train**  Logical vector with TRUE for the training samples and FALSE for the test samples

Source

Index

*Topic classification
  cppls.fit, 8

*Topic datasets
  gasoline, 15
  mayonnaise, 19
  oliveoil, 30
  yarn, 56

*Topic hplot
  biplot.mvr, 2
  coefplot, 6
  plot.mvr, 32
  predplot, 37
  scoreplot, 39
  validationplot, 50

*Topic htest
  jack.test, 16

*Topic models
  cvsegments, 14

*Topic multivariate
  biplot.mvr, 2
  coef.mvr, 4
  coefplot, 6
  cppls.fit, 8
  crossval, 11
  kernelpls.fit, 18
  msc, 20
  mvr, 21
  mvrCv, 25
  mvrVal, 28
  oscorespls.fit, 31
  plot.mvr, 32
  pls.options, 33
  predict.mvr, 35
  predplot, 37
  scoreplot, 39
  scores, 42
  selectNcomp, 43
  simpls.fit, 45
  stdize, 47
  summary.mvr, 48
  svdpc.fit, 49
  validationplot, 50
  widekernelpls.fit, 54

*Topic regression
  biplot.mvr, 2
  coef.mvr, 4
  coefplot, 6
  cppls.fit, 8
  crossval, 11
  kernelpls.fit, 18
  msc, 20
  mvr, 21
  mvrCv, 25
  mvrVal, 28
  oscorespls.fit, 31
  plot.mvr, 32
  pls.options, 33
  predict.mvr, 35
  predplot, 37
  scoreplot, 39
  scores, 42
  selectNcomp, 43
  simpls.fit, 45
  stdize, 47
  summary.mvr, 48
  svdpc.fit, 49
  validationplot, 50
  widekernelpls.fit, 54

*Topic univar
  var.jack, 53

  biplot.default, 3
  biplot.mvr, 2, 33

  coef, 4, 5
  coef.mvr, 4, 6, 8, 24, 36, 43
  coefplot, 6, 33
  compnames(coef.mvr), 4
  corrplot, 33

  summary.mvr, 48
  svdpc.fit, 49
  validationplot, 50
  widekernelpls.fit, 54
INDEX

9

crossval, 10, 19, 22, 24

cppls (mv), 19, 34, 50, 56
cppls (mv), 21

cppls.fit, 8, 22, 24
crossval, 11, 23, 24, 26, 27, 30
cvsegments, 12, 13, 14, 26, 27

explvar, 43

explvar (coef.mvr), 4

fitted, 4, 5

fitted.mvr (coef.mvr), 4

gasoline, 15

identify, 40–42

jul.test, 12, 13, 16, 26, 27, 54

kernelpls.fit, 18, 24, 32, 46, 55, 56

legend, 8, 41, 42, 52

lm, 22, 23

loading.weights, 24

loading.weights (scores), 42

loadingsplot, 33

loadingsplot (scoreplot), 39

loadings, 5, 24, 40, 42, 43

loadings (scores), 42

locator, 7, 40, 51

makeCluster, 34

makepredictcall, 20, 47

makepredictcall.msc (msc), 20

makepredictcall.stdized (stdize), 47

matplot, 52

mayonnaise, 19

mclapply, 34

model.frame, 5

model.frame.mvr (coef.mvr), 4

model.matrix, 5

model.matrix.mvr (coef.mvr), 4

msc, 20, 48

MSEP, 13, 24, 27, 49, 51, 52

MSEP (mv), 28

mv, 3, 5, 8, 10, 13, 19, 21, 27, 30, 32–34,

36, 38, 42, 43, 45, 46, 48–50, 52, 56

mvCv, 13, 17, 22–24, 25, 30, 34, 54

mvVal, 28

mvVal stats (mv), 28

na.exclude, 22

na.fail, 22

na.omit, 5, 22, 35

oliveoil, 30

options, 5, 22

oscorespls.fit, 10, 19, 22, 24, 31, 46, 56

par, 7, 37, 38, 40, 51, 52

parallel, 12, 23, 26, 34

parLapply, 34

pcr, 10, 19, 21, 32, 34, 46, 48–50, 56

pcr (mv), 21

plot, 6, 8, 37, 40, 51

plot.loadings (scoreplot), 39

plot.mvr, 3, 8, 24, 32, 36, 38, 41, 42, 52

plot.mvrVal, 30

plot.mvrVal (validationplot), 50

plot.scores (scoreplot), 39

pls.options, 12, 23, 26, 33

plsr, 10, 19, 21, 32, 34, 46, 48–50, 56

plsr (mv), 21

points, 7, 40, 51

predict.msc (msc), 20

predict.mvr, 23, 24, 35

predict.stdized (stdize), 47

prednames (coef.mvr), 4

predplot, 36, 37

predplot.mvr, 33

predplot.xy (predplot), 37

print.jacktest (jack.test), 16

print.mvr (summary.mvr), 48

print.mvrVal (summary.mvr), 48

printCoefmat, 16

R2, 24, 36, 51, 52

R2 (mv), 28

residuals, 4, 5

residuals.mvr (coef.mvr), 4

respnames (coef.mvr), 4

RMSEP, 24, 36, 49, 51, 52

RMSEP (mv), 28

scale, 47, 48

scoreplot, 33, 39

scores, 5, 24, 40, 42, 42

selectNcomp, 43

simpls.fit, 10, 19, 24, 32, 45, 55, 56

sm.options, 34
stdize, 21, 47
stopCluster, 34
summary.mvr, 36, 45, 48
svdpc.fit, 24, 49

title, 7, 37, 40, 51

validationplot, 30, 33, 50
var.jack, 12, 13, 16, 17, 26, 27, 53

widekernelpls.fit, 10, 19, 22, 24, 32, 46, 54

yarn, 56
Yloadings, 5
Yloadings(scores), 42
Yscores(scores), 42