# Package 'plsRglm'

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Title Partial Least Squares Regression for Generalized Linear Models
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Provides (weighted) Partial least squares Regression for generalized linear models and repeated k fold cross-validation of such models using various criteria. It allows for missing data in the explanatory variables. Bootstrap confidence intervals constructions are also available.
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# **Description**

This function computes the Akaike and Bayesian Information Criteria and the Generalized minimum description length.

# Usage

```
aic.dof(RSS, n, DoF, sigmahat)
bic.dof(RSS, n, DoF, sigmahat)
gmdl.dof(sigmahat, n, DoF, yhat)
```

## **Arguments**

RSS vector of residual sum of squares.

n number of observations.

vector of Degrees of Freedom. The length of DoF is the same as the length of DoF

sigmahat Estimated model error. The length of sigmahat is the same as the length of RSS. vector of squared norm of Yhat. The length of yhat is the same as the length of yhat

sigmahat.

## **Details**

The gmdl criterion is defined as

$$gmdl = \frac{n}{2}log(S) + \frac{DoF}{2}log(F) + \frac{1}{2}log(n)$$

with

$$S = \hat{\sigma}^2$$

#### Value

numerical values of the requested AIC, BIC or GMDL. vector

# Author(s)

```
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```

```
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```

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#### References

M. Hansen, B. Yu. (2001). Model Selection and Minimum Descripion Length Principle, *Journal of the American Statistical Association*, 96, 746-774.

N. Kraemer, M. Sugiyama. (2011). The Degrees of Freedom of Partial Least Squares Regression. *Journal of the American Statistical Association*, 106(494), 697-705.

N. Kraemer, M.L. Braun, Kernelizing PLS, Degrees of Freedom, and Efficient Model Selection, *Proceedings of the 24th International Conference on Machine Learning*, Omni Press, (2007) 441-448.

#### See Also

plsR.dof for degrees of freedom computation and infcrit.dof for computing information criteria directly from a previously fitted plsR model.

## **Examples**

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
modpls <- plsR(yCornell, XCornell, 4)
dof.object <- plsR.dof(modpls)
aic.dof(modpls$RSS,modpls$nr,dof.object$DoF,dof.object$sigmahat)
bic.dof(modpls$RSS,modpls$nr,dof.object$DoF,dof.object$sigmahat)
gmdl.dof(dof.object$sigmahat,modpls$nr,dof.object$DoF,dof.object$yhat)
naive.object <- plsR.dof(modpls,naive=TRUE)
aic.dof(modpls$RSS,modpls$nr,naive.object$DoF,naive.object$sigmahat)
bic.dof(modpls$RSS,modpls$nr,naive.object$DoF,naive.object$sigmahat)
gmdl.dof(naive.object$sigmahat,modpls$nr,naive.object$DoF,naive.object$yhat)</pre>
```

AICpls

AIC function for plsR models

## **Description**

This function provides AIC computation for an univariate plsR model.

# Usage

```
AICpls(ncomp, residpls, weights=rep.int(1,length(residpls)))
```

# **Arguments**

ncomp Number of components

residpls Residuals of a fitted univariate plsR model

weights Weights of observations

#### **Details**

AIC function for plsR models with univariate response.

#### Value

real AIC value

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#### Author(s)

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```

#### References

Baibing Li, Julian Morris, Elaine B. Martin, Model selection for partial least squares regression, Chemometrics and Intelligent Laboratory Systems 64 (2002) 79-89. http://dx.doi.org/10.1016/S0169-7439(02)00051-5

#### See Also

loglikpls for loglikelihood computations for plsR models and AIC for AIC computation for a linear models

# **Examples**

```
data(pine)
ypine <- pine[,11]</pre>
Xpine <- pine[,1:10]</pre>
(Pinscaled <- as.data.frame(cbind(scale(ypine), scale(as.matrix(Xpine)))))</pre>
colnames(Pinscaled)[1] <- "yy"</pre>
lm(yy^x1+x2+x3+x4+x5+x6+x7+x8+x9+x10, data=Pinscaled)
modpls <- plsR(ypine, Xpine, 10)</pre>
modpls$Std.Coeffs
lm(yy^{-}x1+x2+x3+x4+x5+x6+x7+x8+x9+x10, data=Pinscaled)\\
AIC(lm(yy\sim x1+x2+x3+x4+x5+x6+x7+x8+x9+x10,data=Pinscaled))
print(logLik(lm(yy\sim x1+x2+x3+x4+x5+x6+x7+x8+x9+x10, data=Pinscaled)))
sum(dnorm(modpls$RepY, modpls$Std.ValsPredictY, sqrt(mean(modpls$residY^2)), log=TRUE))
sum(dnorm(Pinscaled\$yy,fitted(lm(yy~x1+x2+x3+x4+x5+x6+x7+x8+x9+x10,data=Pinscaled)),
sqrt(mean(residuals(lm(yy\sim x1+x2+x3+x4+x5+x6+x7+x8+x9+x10,data=Pinscaled))^2)), log=TRUE))
loglikpls(modpls$residY)
loglikpls(residuals(lm(yy^x1+x2+x3+x4+x5+x6+x7+x8+x9+x10,data=Pinscaled)))\\
AICpls(10, residuals(lm(yy^x1+x2+x3+x4+x5+x6+x7+x8+x9+x10, data=Pinscaled)))
AICpls(10, modpls$residY)
```

aze

Microsatellites Dataset

# Description

This database was collected on patients carrying a colon adenocarcinoma. It has 104 observations on 33 binary qualitative explanatory variables and one response variable y representing the cancer stage according to the to Astler-Coller classification (Astler and Coller, 1954). This dataset has some missing data due to technical limits. A microsattelite is a non-coding DNA sequence.

#### Usage

```
data(aze)
```

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#### **Format**

A data frame with 104 observations on the following 34 variables.

y the response: a binary vector (Astler-Coller score). D2S138 a binary vector that indicates whether this microsatellite is altered or not. D18S61 a binary vector that indicates whether this microsatellite is altered or not. D16S422 a binary vector that indicates whether this microsatellite is altered or not. D17S794 a binary vector that indicates whether this microsatellite is altered or not. D6S264 a binary vector that indicates whether this microsatellite is altered or not. D14S65 a binary vector that indicates whether this microsatellite is altered or not. D18S53 a binary vector that indicates whether this microsatellite is altered or not. D17S790 a binary vector that indicates whether this microsatellite is altered or not. D1S225 a binary vector that indicates whether this microsatellite is altered or not. D3S1282 a binary vector that indicates whether this microsatellite is altered or not. D9S179 a binary vector that indicates whether this microsatellite is altered or not. D5S430 a binary vector that indicates whether this microsatellite is altered or not. D8S283 a binary vector that indicates whether this microsatellite is altered or not. D11S916 a binary vector that indicates whether this microsatellite is altered or not. D2S159 a binary vector that indicates whether this microsatellite is altered or not. D16S408 a binary vector that indicates whether this microsatellite is altered or not. D5S346 a binary vector that indicates whether this microsatellite is altered or not. D10S191 a binary vector that indicates whether this microsatellite is altered or not. D13S173 a binary vector that indicates whether this microsatellite is altered or not. D6S275 a binary vector that indicates whether this microsatellite is altered or not. D15S127 a binary vector that indicates whether this microsatellite is altered or not. D1S305 a binary vector that indicates whether this microsatellite is altered or not. D4S394 a binary vector that indicates whether this microsatellite is altered or not. D20S107 a binary vector that indicates whether this microsatellite is altered or not. D1S197 a binary vector that indicates whether this microsatellite is altered or not. D1S207 a binary vector that indicates whether this microsatellite is altered or not. D10S192 a binary vector that indicates whether this microsatellite is altered or not. D3S1283 a binary vector that indicates whether this microsatellite is altered or not. D4S414 a binary vector that indicates whether this microsatellite is altered or not. D8S264 a binary vector that indicates whether this microsatellite is altered or not. D22S928 a binary vector that indicates whether this microsatellite is altered or not. TP53 a binary vector that indicates whether this microsatellite is altered or not. D9S171 a binary vector that indicates whether this microsatellite is altered or not.

#### **Source**

Weber *et al.* (2007). Allelotyping analyzes of synchronous primary and metastasis CIN colon cancers identified different subtypes. *Int J Cancer*, 120(3), pages 524-32.

aze\_compl 7

#### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18.

#### **Examples**

data(aze)
str(aze)

aze\_compl

As aze without missing values

# **Description**

This is a single imputation of the aze dataset which was collected on patients carrying a colon adenocarcinoma. It has 104 observations on 33 binary qualitative explanatory variables and one response variable y representing the cancer stage according to the to Astler-Coller classification (Astler and Coller, 1954). A microsattelite is a non-coding DNA sequence.

#### Usage

```
data(aze_compl)
```

#### **Format**

A data frame with 104 observations on the following 34 variables.

y the response: a binary vector (Astler-Coller score).

D2S138 a binary vector that indicates whether this microsatellite is altered or not.

D18S61 a binary vector that indicates whether this microsatellite is altered or not.

D16S422 a binary vector that indicates whether this microsatellite is altered or not.

D17S794 a binary vector that indicates whether this microsatellite is altered or not.

D6S264 a binary vector that indicates whether this microsatellite is altered or not. D14S65 a binary vector that indicates whether this microsatellite is altered or not.

D18S53 a binary vector that indicates whether this microsatellite is altered or not.

D17S790 a binary vector that indicates whether this microsatellite is altered or not.

D1S225 a binary vector that indicates whether this microsatellite is altered or not.

D3S1282 a binary vector that indicates whether this microsatellite is altered or not.

D9S179 a binary vector that indicates whether this microsatellite is altered or not.

D5S430 a binary vector that indicates whether this microsatellite is altered or not.

D8S283 a binary vector that indicates whether this microsatellite is altered or not.

D11S916 a binary vector that indicates whether this microsatellite is altered or not.

D2S159 a binary vector that indicates whether this microsatellite is altered or not.

D16S408 a binary vector that indicates whether this microsatellite is altered or not.

D5S346 a binary vector that indicates whether this microsatellite is altered or not.

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D10S191 a binary vector that indicates whether this microsatellite is altered or not. D13S173 a binary vector that indicates whether this microsatellite is altered or not. D6S275 a binary vector that indicates whether this microsatellite is altered or not. D15S127 a binary vector that indicates whether this microsatellite is altered or not. D1S305 a binary vector that indicates whether this microsatellite is altered or not. D4S394 a binary vector that indicates whether this microsatellite is altered or not. D20S107 a binary vector that indicates whether this microsatellite is altered or not. D1S197 a binary vector that indicates whether this microsatellite is altered or not. D1S207 a binary vector that indicates whether this microsatellite is altered or not. D10S192 a binary vector that indicates whether this microsatellite is altered or not. D3S1283 a binary vector that indicates whether this microsatellite is altered or not. D4S414 a binary vector that indicates whether this microsatellite is altered or not. D8S264 a binary vector that indicates whether this microsatellite is altered or not. D22S928 a binary vector that indicates whether this microsatellite is altered or not. TP53 a binary vector that indicates whether this microsatellite is altered or not. D9S171 a binary vector that indicates whether this microsatellite is altered or not.

#### **Source**

Weber *et al.* (2007). Allelotyping analyzes of synchronous primary and metastasis CIN colon cancers identified different subtypes. *Int J Cancer*, 120(3), pages 524-32.

#### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18.

## **Examples**

```
data(aze_compl)
str(aze_compl)
```

bootpls

Non-parametric Bootstrap for PLS models

#### **Description**

Provides a wrapper for the bootstrap function boot from the boot R package. Implements non-parametric bootstraps for PLS Regression models by either (Y,X) or (Y,T) resampling.

#### Usage

```
bootpls(object, typeboot="plsmodel", R=250, statistic=coefs.plsR, sim="ordinary",
stype="i", stabvalue=1e6, verbose=TRUE,...)
```

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#### **Arguments**

object An object of class plsRmodel to bootstrap typeboot The type of bootstrap. Either (Y,X) boostrap (typeboot="plsmodel") or (Y,T) bootstrap (typeboot="fmodel\_np"). Defaults to (Y,X) resampling. R The number of bootstrap replicates. Usually this will be a single positive integer. For importance resampling, some resamples may use one set of weights and others use a different set of weights. In this case R would be a vector of integers where each component gives the number of resamples from each of the rows of weights. statistic A function which when applied to data returns a vector containing the statistic(s) of interest. statistic must take at least two arguments. The first argument passed will always be the original data. The second will be a vector of indices, frequencies or weights which define the bootstrap sample. Further, if predictions are required, then a third argument is required which would be a vector of the random indices used to generate the bootstrap predictions. Any further arguments can be passed to statistic through the . . . argument. sim A character string indicating the type of simulation required. Possible values are "ordinary" (the default), "balanced", "permutation", or "antithetic". A character string indicating what the second argument of statistic represtype sents. Possible values of stype are "i" (indices - the default), "f" (frequencies), or "w" (weights). stabvalue A value to hard threshold bootstrap estimates computed from atypical resamplings. Especially useful for Generalized Linear Models. verbose should info messages be displayed?

.. Other named arguments for statistic which are passed unchanged each time it

is called. Any such arguments to statistic should follow the arguments which statistic is required to have for the simulation. Beware of partial matching to

arguments of boot listed above.

#### Details

More details on bootstrap techniques are available in the help of the boot function.

#### Value

An object of class "boot". See the Value part of the help of the function boot.

#### Author(s)

```
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http://www-irma.u-strasbg.fr/~fbertran/
```

#### References

A. Lazraq, R. Cleroux, and J.-P. Gauchi. (2003). Selecting both latent and explanatory variables in the PLS1 regression model. *Chemometrics and Intelligent Laboratory Systems*, 66(2):117-126. P. Bastien, V. Esposito-Vinzi, and M. Tenenhaus. (2005). PLS generalised linear regression. *Computational Statistics & Data Analysis*, 48(1):17-46.

A. C. Davison and D. V. Hinkley. (1997). *Bootstrap Methods and Their Applications*. Cambridge University Press, Cambridge.

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#### See Also

boot

```
data(Cornell)
XCornell<-Cornell[,1:7]</pre>
yCornell<-Cornell[,8]
# Lazraq-Cleroux PLS ordinary bootstrap
set.seed(250)
modpls <- plsR(yCornell, XCornell, 3)</pre>
#(Y,X) resampling
Cornell.bootYX <- bootpls(modpls, R=250)</pre>
#(Y,T) resampling
Cornell.bootYT <- bootpls(modpls, typeboot="fmodel_np", R=250)</pre>
# Using the boxplots.bootpls function
boxplots.bootpls(Cornell.bootYX,indices=2:8)
# Confidence intervals plotting
confints.bootpls(Cornell.bootYX,indices=2:8)
plots.confints.bootpls(confints.bootpls(Cornell.bootYX,indices=2:8))
# Graph similar to the one of Bastien et al. in CSDA 2005
boxplot(as.vector(Cornell.bootYX$t[,-1])~factor(rep(1:7,rep(250,7))),
main="Bootstrap distributions of standardised bj (j = 1, ..., 7).")
points(c(1:7),Cornell.bootYX$t0[-1],col="red",pch=19)
library(boot)
boot.ci(Cornell.bootYX, conf = c(0.90,0.95), type = c("norm","basic","perc","bca"), index=2)
plot(Cornell.bootYX,index=2)
jack.after.boot(Cornell.bootYX, index=2, useJ=TRUE, nt=3)
plot(Cornell.bootYX,index=2,jack=TRUE)
car::dataEllipse(Cornell.bootYX$t[,2], Cornell.bootYX$t[,3], cex=.3,
levels=c(.5, .95, .99), robust=TRUE)
rm(Cornell.bootYX)
# PLS balanced bootstrap
set.seed(225)
Cornell.bootYX <- bootpls(modpls, sim="balanced", R=250)</pre>
boot.array(Cornell.bootYX, indices=TRUE)
# Using the boxplots.bootpls function
boxplots.bootpls(Cornell.bootYX,indices=2:8)
# Confidence intervals plotting
confints.bootpls(Cornell.bootYX,indices=2:8)
plots.confints.bootpls(confints.bootpls(Cornell.bootYX,indices=2:8))
# Graph similar to the one of Bastien et al. in CSDA 2005
boxplot(as.vector(Cornell.bootYX$t[,-1])~factor(rep(1:7,rep(250,7))),
main="Bootstrap distributions of standardised bj (j = 1, ..., 7).")
```

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```
points(c(1:7),Cornell.bootYX$t0[-1],col="red",pch=19)
library(boot)
boot.ci(Cornell.bootYX, conf = c(0.90,0.95), type = c("norm", "basic", "perc", "bca"), index=2)
plot(Cornell.bootYX,index=2)
jack.after.boot(Cornell.bootYX, index=2, useJ=TRUE, nt=3)
plot(Cornell.bootYX,index=2,jack=TRUE)
rm(Cornell.bootYX)
# PLS permutation bootstrap
set.seed(500)
Cornell.bootYX <- bootpls(modpls, sim="permutation", R=1000)</pre>
boot.array(Cornell.bootYX, indices=TRUE)
# Graph of bootstrap distributions
boxplot(as.vector(Cornell.bootYX$t[,-1])~factor(rep(1:7,rep(1000,7))),
main="Bootstrap distributions of standardised bj (j = 1, ..., 7).")
points(c(1:7),Cornell.bootYX$t0[-1],col="red",pch=19)
# Using the boxplots.bootpls function
boxplots.bootpls(Cornell.bootYX,indices=2:8)
library(boot)
plot(Cornell.bootYX,index=2)
qqnorm(Cornell.bootYX$t[,2],ylim=c(-1,1))
abline(h=Cornell.bootYX$t0[2],lty=2)
(sum(abs(Cornell.bootYX$t[,2])>=abs(Cornell.bootYX$t0[2]))+1)/(length(Cornell.bootYX$t[,2])+1)
rm(Cornell.bootYX)
```

bootplsglm

Non-parametric Bootstrap for PLS generalized linear models

#### **Description**

Provides a wrapper for the bootstrap function boot from the boot R package. Implements non-parametric bootstraps for PLS Generalized Linear Regression models by either (Y,X) or (Y,T) resampling.

## Usage

```
bootplsglm(object, typeboot="fmodel_np", R=250, statistic=coefs.plsRglmnp,
sim="ordinary", stype="i", stabvalue=1e6, verbose=TRUE,...)
```

#### **Arguments**

object

An object of class plsRglmmodel to bootstrap

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typeboot The type of bootstrap. Either (Y,X) boostrap (typeboot="plsmodel") or (Y,T) bootstrap (typeboot="fmodel\_np"). Defaults to (Y,T) resampling.

R The number of bootstrap replicates. Usually this will be a single positive integer.

For importance resampling, some resamples may use one set of weights and others use a different set of weights. In this case R would be a vector of integers where each component gives the number of resamples from each of the rows of

weights.

statistic A function which when applied to data returns a vector containing the statistic(s)

of interest. statistic must take at least two arguments. The first argument passed will always be the original data. The second will be a vector of indices, frequencies or weights which define the bootstrap sample. Further, if predictions are required, then a third argument is required which would be a vector of the random indices used to generate the bootstrap predictions. Any further

arguments can be passed to statistic through the . . . argument.

sim A character string indicating the type of simulation required. Possible values are

"ordinary" (the default), "balanced", "permutation", or "antithetic".

stype A character string indicating what the second argument of statistic repre-

sents. Possible values of stype are "i" (indices - the default), "f" (frequencies),

or "w" (weights).

stabvalue A value to hard threshold bootstrap estimates computed from atypical resam-

plings. Especially useful for Generalized Linear Models.

verbose should info messages be displayed?

... Other named arguments for statistic which are passed unchanged each time it

is called. Any such arguments to statistic should follow the arguments which statistic is required to have for the simulation. Beware of partial matching to

arguments of boot listed above.

#### **Details**

More details on bootstrap techniques are available in the help of the boot function.

## Value

An object of class "boot". See the Value part of the help of the function boot.

#### Author(s)

Frederic Bertrand

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#### References

A. Lazraq, R. Cleroux, and J.-P. Gauchi. (2003). Selecting both latent and explanatory variables in the PLS1 regression model. *Chemometrics and Intelligent Laboratory Systems*, 66(2):117-126. P. Bastien, V. Esposito-Vinzi, and M. Tenenhaus. (2005). PLS generalised linear regression. *Computational Statistics & Data Analysis*, 48(1):17-46.

A. C. Davison and D. V. Hinkley. (1997). *Bootstrap Methods and Their Applications*. Cambridge University Press, Cambridge.

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#### See Also

boot

```
#Imputed aze dataset
data(aze_compl)
Xaze_compl<-aze_compl[,2:34]</pre>
yaze_compl<-aze_compl$y</pre>
dataset <- cbind(y=yaze_compl, Xaze_compl)</pre>
modplsglm \leftarrow plsRglm(y^{-}, data=dataset, 3, modele="pls-glm-logistic")
library(boot)
# Bastien (Y,T) PLS bootstrap
aze_compl.bootYT <- bootplsglm(modplsglm, R=250)</pre>
boxplots.bootpls(aze_compl.bootYT)
confints.bootpls(aze_compl.bootYT)
plots.confints.bootpls(confints.bootpls(aze_compl.bootYT))
plot(aze_compl.bootYT,index=2)
jack.after.boot(aze_compl.bootYT, index=2, useJ=TRUE, nt=3)
plot(aze_compl.bootYT, index=2,jack=TRUE)
aze_compl.tilt.boot <- tilt.bootplsglm(modplsglm, statistic=coefs.plsRglm,</pre>
R=c(499, 100, 100), alpha=c(0.025, 0.975), sim="ordinary", stype="i", index=1)
# PLS bootstrap balanced
aze_compl.bootYT <- bootplsglm(modplsglm, sim="balanced", R=250)</pre>
boxplots.bootpls(aze_compl.bootYT)
confints.bootpls(aze_compl.bootYT)
plots.confints.bootpls(confints.bootpls(aze_compl.bootYT))
plot(aze_compl.bootYT)
jack.after.boot(aze_compl.bootYT, index=1, useJ=TRUE, nt=3)
plot(aze_compl.bootYT, jack=TRUE)
aze_compl.tilt.boot <- tilt.bootplsglm(modplsglm, statistic=coefs.plsR,</pre>
R=c(499, 100, 100), alpha=c(0.025, 0.975), sim="balanced", stype="i", index=1)
# PLS permutation bootstrap
aze_compl.bootYT <- bootplsglm(modplsglm, sim="permutation", R=250)</pre>
boxplots.bootpls(aze_compl.bootYT)
plot(aze_compl.bootYT)
#Original aze dataset with missing values
data(aze)
Xaze<-aze[,2:34]
yaze<-aze$y
library(boot)
modplsglm2 <- plsRglm(yaze, Xaze, 3, modele="pls-glm-logistic")</pre>
aze.bootYT <- bootplsglm(modplsglm2, R=250)</pre>
```

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```
boxplots.bootpls(aze.bootYT)
confints.bootpls(aze.bootYT)
plots.confints.bootpls(confints.bootpls(aze.bootYT))
#Ordinal logistic regression
data(bordeaux)
Xbordeaux<-bordeaux[,1:4]
ybordeaux<-factor(bordeaux$Quality,ordered=TRUE)</pre>
dataset <- cbind(y=ybordeaux, Xbordeaux)</pre>
options(contrasts = c("contr.treatment", "contr.poly"))
modplsglm3 <- plsRglm(ybordeaux, Xbordeaux, 1, modele="pls-glm-polr")</pre>
bordeaux.bootYT<- bootplsglm(modplsglm3, sim="permutation", R=250)</pre>
boxplots.bootpls(bordeaux.bootYT)
boxplots.bootpls(bordeaux.bootYT,ranget0=TRUE)
bordeaux.bootYT2<- bootplsglm(modplsglm3, sim="permutation", R=250,</pre>
strata=unclass(ybordeaux))
boxplots.bootpls(bordeaux.bootYT2,ranget0=TRUE)
if(require(chemometrics)){
data(hyptis)
hyptis
yhyptis <- factor(hyptis$Group,ordered=TRUE)</pre>
Xhyptis <- as.data.frame(hyptis[,c(1:6)])</pre>
dataset <- cbind(y=yhyptis, Xhyptis)</pre>
options(contrasts = c("contr.treatment", "contr.poly"))
modplsglm4 <- plsRglm(yhyptis, Xhyptis, 3, modele="pls-glm-polr")</pre>
hyptis.bootYT3<- bootplsglm(modplsglm4, sim="permutation", R=250)</pre>
rownames(hyptis.bootYT3$t0)<-c("Sabi\nnene", "Pin\nene",</pre>
"Cine\nole", "Terpi\nnene", "Fenc\nhone", "Terpi\nnolene")
boxplots.bootpls(hyptis.bootYT3)
boxplots.bootpls(hyptis.bootYT3,xaxisticks=FALSE)
boxplots.bootpls(hyptis.bootYT3,ranget0=TRUE)
boxplots.bootpls(hyptis.bootYT3,ranget0=TRUE,xaxisticks=FALSE)
}
```

bordeaux

Quality of wine dataset

#### Description

Quality of Bordeaux wines (Quality) and four potentially predictive variables (Temperature, Sunshine, Heat and Rain).

# Usage

```
data(bordeaux)
```

boxplots.bootpls 15

#### **Format**

A data frame with 34 observations on the following 5 variables.

```
Temperature a numeric vector

Sunshine a numeric vector

Heat a numeric vector

Rain a numeric vector

Quality an ordered factor with levels 1 < 2 < 3
```

#### **Source**

P. Bastien, V. Esposito-Vinzi, and M. Tenenhaus. (2005). PLS generalised linear regression. *Computational Statistics & Data Analysis*, 48(1):17-46.

#### References

M. Tenenhaus. (2005). La regression logistique PLS. In J.-J. Droesbeke, M. Lejeune, and G. Saporta, editors, Modeles statistiques pour données qualitatives. Editions Technip, Paris.

# **Examples**

```
data(bordeaux)
str(bordeaux)
```

boxplots.bootpls

Boxplot bootstrap distributions

# Description

Boxplots for bootstrap distributions.

#### Usage

```
boxplots.bootpls(bootobject, indices = NULL, prednames = TRUE,
articlestyle = TRUE, xaxisticks=TRUE, ranget0= FALSE, las = par("las"),
mar, mgp, ...)
```

# Arguments

bootobject	a object of class "boot"
indices	vector of indices of the variables to plot. Defaults to NULL: all the predictors will be used.
prednames	do the original names of the predictors shall be plotted ? Defaults to TRUE: the names are plotted.
articlestyle	do the extra blank zones of the margin shall be removed from the plot? Defaults to TRUE: the margins are removed.
xaxisticks	do ticks for the x axis shall be plotted? Defaults to TRUE: the ticks are plotted.

boxplots.bootpls

ranget0	does the vertival range of the plot shall be computed to include the initial estimates of the coefficients? Defaults to FALSE: the vertical range is calculated only using the bootstrapped values of the statistics. Especially using for permutation bootstrap.
las	numeric in 0,1,2,3; the style of axis labels. 0: always parallel to the axis [default], 1: always horizontal, 2: always perpendicular to the axis, 3: always vertical.
mar	A numerical vector of the form $c(bottom, left, top, right)$ which gives the number of lines of margin to be specified on the four sides of the plot. The default is $c(5, 4, 4, 2) + 0.1$ .
mgp	The margin line (in mex units) for the axis title, axis labels and axis line. Note that $mgp[1]$ affects title whereas $mgp[2:3]$ affect axis. The default is $c(3, 1, 0)$ .
	further options to pass to the boxplot function.

## Value

NULL

# Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

## See Also

bootpls

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]

# Lazraq-Cleroux PLS ordinary bootstrap
set.seed(250)
modpls <- plsR(yCornell,XCornell,3)
Cornell.bootYX <- bootpls(modpls, R=250)

# Graph similar to the one of Bastien et al. in CSDA 2005
boxplots.bootpls(Cornell.bootYX,indices=2:8)

data(aze_compl)
modplsglm<-plsRglm(y~.,data=aze_compl,3,modele="pls-glm-logistic")
aze_compl.boot3 <- bootplsglm(modplsglm, R=250)
boxplots.bootpls(aze_compl.boot3)
boxplots.bootpls(aze_compl.boot3,las=3,mar=c(5,2,1,1))
boxplots.bootpls(aze_compl.boot3,indices=c(2,4,6),prednames=FALSE)</pre>
```

coef.plsRglmmodel 17

coef.plsRglmmodel

coef method for plsR models

## **Description**

This function provides a coef method for the class "plsRglmmodel"

#### Usage

```
## S3 method for class 'plsRglmmodel'
coef(object,type=c("scaled","original"), ...)
```

#### **Arguments**

object an object of the class "plsRglmmodel"

type if scaled, the coefficients of the predictors are given for the scaled predictors,

if original the coefficients are to be used with the predictors on their original

scale.

... not used

#### Value

An object of class coef.plsRglmmodel.

CoeffC Coefficients of the components.

Std.Coeffs Coefficients of the scaled predictors in the regression function.

Coeffs Coefficients of the untransformed predictors (on their original scale).

# Author(s)

```
Frederic Bertrand
```

```
<frederic.bertrand@math.unistra.fr>
http://www-irma.u-strasbg.fr/~fbertran/
```

#### See Also

coef

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
modpls <- plsRglm(yCornell, XCornell, 3, modele="pls-glm-family", family=gaussian())
class(modpls)
coef(modpls)
coef(modpls, type="scaled")
rm(list=c("XCornell", "yCornell", "modpls"))</pre>
```

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coef.plsRmodel

coef method for plsR models

## **Description**

This function provides a coef method for the class "plsRmodel"

#### Usage

```
## S3 method for class 'plsRmodel'
coef(object,type=c("scaled","original"), ...)
```

## **Arguments**

object an object of the class "plsRmodel"

type if scaled, the coefficients of the predictors are given for the scaled predictors,

if original the coefficients are to be used with the predictors on their original

scale.

... not used

#### Value

An object of class coef.plsRmodel.

CoeffC Coefficients of the components.

Std.Coeffs Coefficients of the scaled predictors.

Coeffs Coefficients of the untransformed predictors (on their original scale).

# Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

#### See Also

coef

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
modpls <- plsRglm(yCornell, XCornell, 3, modele="pls")
class(modpls)
coef(modpls)
coef(modpls, type="scaled")
rm(list=c("XCornell", "yCornell", "modpls"))</pre>
```

coefs.plsR

coefs.plsR	Coefficients for bootstrap computations of PLSR models
------------	--

## **Description**

A function passed to boot to perform bootstrap.

# Usage

```
coefs.plsR(dataset,ind,nt,modele, maxcoefvalues,ifbootfail,verbose)
```

# **Arguments**

dataset dataset to resample
ind indices for resampling
nt number of components to use

modele type of modele to use, see plsR

maxcoefvalues maximum values allowed for the estimates of the coefficients to discard those

coming from singular bootstrap samples

ifbootfail value to return if the estimation fails on a bootstrap sample

verbose should info messages be displayed?

## Value

estimates on a bootstrap sample or ifbootfail value if the bootstrap computation fails.

#### Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

# See Also

See also bootpls.

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]

# Lazraq-Cleroux PLS (Y,X) bootstrap
# statistic=coefs.plsR is the default for (Y,X) resampling of PLSR models.
set.seed(250)
modpls <- plsR(yCornell,XCornell,1)
Cornell.bootYX <- bootpls(modpls, R=250, statistic=coefs.plsR)</pre>
```

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coefs.plsRglm	Coefficients for bootstrap computations of PLSGLR models	
---------------	--	--

## **Description**

A function passed to boot to perform bootstrap.

# Usage

```
coefs.plsRglm(dataset, ind, nt, modele, family=NULL, maxcoefvalues,ifbootfail,verbose)
```

## **Arguments**

dataset dataset to resample

ind indices for resampling

nt number of components to use

modele type of modele to use, see plsRglm

family glm family to use, see plsRglm

maxcoefvalues maximum values allowed for the estimates of the coefficients to discard those coming from singular bootstrap samples

ifbootfail value to return if the estimation fails on a bootstrap sample

verbose should info messages be displayed?

#### Value

estimates on a bootstrap sample or ifbootfail value if the bootstrap computation fails.

## Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

#### See Also

See also bootplsglm.

```
data(Cornell)
# (Y,X) bootstrap of a PLSGLR model
# statistic=coefs.plsRglm is the default for (Y,X) bootstrap of a PLSGLR models.
set.seed(250)
modplsglm <- plsRglm(Y~.,data=Cornell,1,modele="pls-glm-family",family=gaussian)
Cornell.bootYX <- bootplsglm(modplsglm, R=250, typeboot="plsmodel", statistic=coefs.plsRglm)</pre>
```

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coefs.plsRglmnp	Coefficients for bootstrap computations	of PLSGLR models
-----------------	---	------------------

## **Description**

A function passed to boot to perform bootstrap.

# Usage

```
coefs.plsRglmnp(dataRepYtt, ind, nt, modele, family=NULL,
maxcoefvalues, wwetoile,ifbootfail)
```

## **Arguments**

dataRepYtt components' coordinates to bootstrap

ind indices for resampling

nt number of components to use
modele type of modele to use, see plsRglm
family glm family to use, see plsRglm

maxcoefvalues maximum values allowed for the estimates of the coefficients to discard those

coming from singular bootstrap samples

wwetoile values of the Wstar matrix in the original fit

ifbootfail value to return if the estimation fails on a bootstrap sample

#### Value

estimates on a bootstrap sample or ifbootfail value if the bootstrap computation fails.

#### Note

```
~~some notes~~
```

#### Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

#### See Also

See also bootplsglm

```
data(Cornell)
# (Y,X) bootstrap of a PLSGLR model
# statistic=coefs.plsRglm is the default for (Y,X) bootstrap of a PLSGLR models.
set.seed(250)
modplsglm <- plsRglm(Y~.,data=Cornell,1,modele="pls-glm-family",family=gaussian)
Cornell.bootYT <- bootplsglm(modplsglm, R=250, statistic=coefs.plsRglmnp)</pre>
```

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coefs.plsRnp	Coefficients for bootstrap computations of PLSR models
--------------	--

## **Description**

A function passed to boot to perform bootstrap.

# Usage

```
coefs.plsRnp(dataRepYtt,ind,nt,modele, maxcoefvalues,wwetoile,ifbootfail)
```

# Arguments

dataRepYtt components' coordinates to bootstrap

ind indices for resampling

nt number of components to use

modele type of modele to use, see plsRglm

maxcoefvalues maximum values allowed for the estimates of the coefficients to discard those

coming from singular bootstrap samples

wwetoile values of the Wstar matrix in the original fit

ifbootfail value to return if the estimation fails on a bootstrap sample

#### Value

estimates on a bootstrap sample or ifbootfail value if the bootstrap computation fails.

#### Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

# See Also

See also bootpls

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]

# Lazraq-Cleroux PLS (Y,X) bootstrap
# statistic=coefs.plsR is the default for (Y,X) resampling of PLSR models.
set.seed(250)
modpls <- plsR(yCornell,XCornell,1)
Cornell.bootYT <- bootpls(modpls, R=250, typeboot="fmodel_np", statistic=coefs.plsRnp)</pre>
```

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confints.bootpls

Bootstrap confidence intervals

#### **Description**

This function is a wrapper for boot.ci to derive bootstrap-based confidence intervals from a "boot" object.

# Usage

```
confints.bootpls(bootobject, indices = NULL, typeBCa=TRUE)
```

#### **Arguments**

bootobject an object of class "boot"

indices the indices of the predictor for which CIs should be calculated. Defaults to NULL:

all the predictors will be used.

typeBCa shall BCa bootstrap based CI derived? Defaults to TRUE. This is a safety op-

tion since sometimes computing BCa bootstrap based CI fails whereas the other

types of CI can still be derived.

## Value

Matrix with the limits of bootstrap based CI for all (defaults) or only the selected predictors (indices option). The limits are given in that order: Normal Lower then Upper Limit, Basic Lower then Upper Limit, Percentile Lower then Upper Limit, BCa Lower then Upper Limit.

#### Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

## See Also

See also bootpls and bootplsglm.

```
data(Cornell)
#Lazraq-Cleroux PLS (Y,X) bootstrap
set.seed(250)
modpls <- plsR(Y~.,data=Cornell,3)
Cornell.bootYX <- bootpls(modpls, R=250)
confints.bootpls(Cornell.bootYX,2:8)
confints.bootpls(Cornell.bootYX,2:8,typeBCa=FALSE)</pre>
```

24 CorMat

CorMat

Correlation matrix for simulating plsR datasets

# Description

A correlation matrix to simulate datasets

# Usage

```
data(CorMat)
```

#### **Format**

A data frame with 17 observations on the following 17 variables.

```
y a numeric vector
```

x11 a numeric vector

x12 a numeric vector

x13 a numeric vector

x21 a numeric vector

x22 a numeric vector

x31 a numeric vector

x32 a numeric vector

x33 a numeric vector

x34 a numeric vector

x41 a numeric vector

x42 a numeric vector

x51 a numeric vector

x61 a numeric vector

x62 a numeric vector

x63 a numeric vector

x64 a numeric vector

## **Source**

Handmade.

# References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

```
data(CorMat)
str(CorMat)
```

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Cornell dataset

# Description

The famous Cornell dataset. A mixture experiment on X1, X2, X3, X4, X5, X6 and X7 to analyse octane degree (Y) in gazoline.

# Usage

```
data(Cornell)
```

#### **Format**

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

X1 a numeric vector

X2 a numeric vector

X3 a numeric vector

X4 a numeric vector

X5 a numeric vector

X6 a numeric vector

X7 a numeric vector

Y response value: a numeric vector

# Source

M. Tenenhaus. (1998). La regression PLS, Theorie et pratique. Editions Technip, Paris.

#### References

N. Kettaneh-Wold. Analysis of mixture data with partial least squares. (1992). *Chemometrics and Intelligent Laboratory Systems*, 14(1):57-69.

```
data(Cornell)
str(Cornell)
```

26 cv.plsR

cv.plsR	Partial least squares regression models with k-fold cross-validation

# Description

This function implements k-fold cross-validation on complete or incomplete datasets for partial least squares regression models

# Usage

```
cv.plsR(x, ...)
## Default S3 method:
cv.plsRmodel(dataY,dataX,nt=2,limQ2set=.0975,modele="pls",
K=5, NK=1, grouplist=NULL, random=TRUE, scaleX=TRUE,
scaleY=NULL, keepcoeffs=FALSE, keepfolds=FALSE, keepdataY=TRUE,
keepMclassed=FALSE, tol_Xi=10^(-12), weights, verbose=TRUE)
## S3 method for class 'formula'
cv.plsRmodel(formula,data=NULL,nt=2,limQ2set=.0975,modele="pls",
K=5, NK=1, grouplist=NULL, random=TRUE, scaleX=TRUE,
scaleY=NULL, keepcoeffs=FALSE, keepfolds=FALSE, keepdataY=TRUE,
keepMclassed=FALSE, tol_Xi=10^(-12), weights, subset, contrasts=NULL, verbose=TRUE)
PLS_lm_kfoldcv(dataY, dataX, nt = 2, limQ2set = 0.0975, modele = "pls",
K = 5, NK = 1, grouplist = NULL, random = TRUE, scaleX = TRUE,
scaleY = NULL, keepcoeffs = FALSE, keepfolds = FALSE, keepdataY = TRUE,
keepMclassed=FALSE, tol_Xi = 10^(-12), weights, verbose=TRUE)
PLS_lm_kfoldcv_formula(formula,data=NULL,nt=2,limQ2set=.0975,modele="pls",
K=5, NK=1, grouplist=NULL, random=TRUE, scaleX=TRUE,
scaleY=NULL, keepcoeffs=FALSE, keepfolds=FALSE, keepdataY=TRUE,
keepMclassed=FALSE, tol_Xi=10^(-12), weights, subset, contrasts=NULL, verbose=TRUE)
```

#### **Arguments**

X	a formula or a response (training) dataset
dataY	response (training) dataset
dataX	predictor(s) (training) dataset
formula	an object of class "formula" (or one that can be coerced to that class): a symbolic description of the model to be fitted. The details of model specification are given under 'Details'.
data	an optional data frame, list or environment (or object coercible by as.data.frame to a data frame) containing the variables in the model. If not found in data, the variables are taken from environment(formula), typically the environment from which plsRglm is called.
nt	number of components to be extracted
limQ2set	limit value for the Q2
modele	name of the PLS model to be fitted, only ("pls" available for this fonction.
K	number of groups. Defaults to 5.
NK	number of times the group division is made
grouplist	to specify the members of the K groups

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random should the K groups be made randomly. Defaults to TRUE scale the predictor(s) : must be set to TRUE for modele="pls" and should be scaleX for glms pls. scaleY scale the response: Yes/No. Ignored since non always possible for glm responses. keepcoeffs shall the coefficients for each model be returned shall the groups' composition be returned keepfolds keepdataY shall the observed value of the response for each one of the predicted value be returned keepMclassed shall the number of miss classed be returned tol\_Xi minimal value for Norm2(Xi) and  $det(pp' \times pp)$  if there is any missing value in the dataX. It defaults to  $10^{-12}$ weights an optional vector of 'prior weights' to be used in the fitting process. Should be NULL or a numeric vector. subset an optional vector specifying a subset of observations to be used in the fitting process. an optional list. See the contrasts.arg of model.matrix.default. contrasts verbose should info messages be displayed? arguments to pass to cv.plsRmodel.default or to cv.plsRmodel.formula . . .

#### **Details**

Predicts 1 group with the K-1 other groups. Leave one out cross validation is thus obtained for K=nrow(dataX).

A typical predictor has the form response ~ terms where response is the (numeric) response vector and terms is a series of terms which specifies a linear predictor for response. A terms specification of the form first + second indicates all the terms in first together with all the terms in second with any duplicates removed.

A specification of the form first:second indicates the set of terms obtained by taking the interactions of all terms in first with all terms in second. The specification first\*second indicates the cross of first and second. This is the same as first + second + first:second.

The terms in the formula will be re-ordered so that main effects come first, followed by the interactions, all second-order, all third-order and so on: to avoid this pass a terms object as the formula.

Non-NULL weights can be used to indicate that different observations have different dispersions (with the values in weights being inversely proportional to the dispersions); or equivalently, when the elements of weights are positive integers w\_i, that each response y\_i is the mean of w\_i unit-weight observations.

#### Value

An object of class "cv.plsRmodel".

results\_kfolds list of NK. Each element of the list sums up the results for a group division:

list of K matrices of size about nrow(dataX)/K \* nt with the predicted values for a growing number of components

•••

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list of K matrices of size about nrow(dataX)/K \* nt with the predicted values for a growing number of components

folds

list of NK. Each element of the list sums up the results for a group division:

list of K vectors of length about nrow(dataX) with the numbers of the rows of dataX that were used as a training set

•••

list of K vectors of length about nrow(dataX) with the numbers of the rows of dataX that were used as a training set

dataY\_kfolds

list of NK. Each element of the list sums up the results for a group division:

list of K matrices of size about nrow(dataX)/K \* 1 with the observed values of the response

•••

list of K matrices of size about nrow(dataX)/K \* 1 with the observed values of the response

the call of the function

#### Note

Work for complete and incomplete datasets.

# Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

## References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

#### See Also

Summary method summary.cv.plsRmodel. kfolds2coeff, kfolds2Pressind, kfolds2Press, kfolds2Mclassedind, kfolds2Mclassed and kfolds2CVinfos\_1m to extract and transform results from k-fold cross-validation.

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]

#Leave one out CV (K=nrow(Cornell)) one time (NK=1)
bbb <- cv.plsR(dataY=yCornell,dataX=XCornell,nt=6,K=nrow(Cornell),NK=1)
bbb2 <- cv.plsR(Y~.,data=Cornell,nt=6,K=12,NK=1)
(sum1<-summary(bbb))

#6-fold CV (K=6) two times (NK=2)
#use random=TRUE to randomly create folds for repeated CV</pre>
```

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```
bbb3 <- cv.plsR(dataY=yCornell,dataX=XCornell,nt=6,K=6,NK=2)
bbb4 <- cv.plsR(Y~.,data=Cornell,nt=6,K=6,NK=2)
(sum3<-summary(bbb3))

cvtable(sum1)
cvtable(sum3)
rm(list=c("XCornell","yCornell","bbb","bbb2","bbb3","bbb4"))</pre>
```

cv.plsRglm

Partial least squares regression glm models with k-fold cross valida-

#### **Description**

This function implements k-fold cross-validation on complete or incomplete datasets for partial least squares regression generalized linear models

## Usage

```
cv.plsRglm(x, ...)
## Default S3 method:
cv.plsRglmmodel(dataY,dataX,nt=2,limQ2set=.0975,
modele="pls", family=NULL, K=5, NK=1, grouplist=NULL, random=TRUE,
scaleX=TRUE, scaleY=NULL, keepcoeffs=FALSE, keepfolds=FALSE,
keepdataY=TRUE, keepMclassed=FALSE, tol_Xi=10^(-12), weights, method,
verbose=TRUE)
## S3 method for class 'formula'
cv.plsRglmmodel(formula,data=NULL,nt=2,limQ2set=.0975,
modele="pls", family=NULL, K=5, NK=1, grouplist=NULL, random=TRUE,
scaleX=TRUE, scaleY=NULL, keepcoeffs=FALSE, keepfolds=FALSE,
keepdataY=TRUE, keepMclassed=FALSE, tol_Xi=10^(-12), weights, subset,
start=NULL,etastart,mustart,offset,method,control= list(),contrasts=NULL,
verbose=TRUE)
PLS_glm_kfoldcv(dataY, dataX, nt = 2, limQ2set = 0.0975, modele = "pls",
family = NULL, K = 5, NK = 1, grouplist = NULL, random = TRUE,
scaleX = TRUE, scaleY = NULL, keepcoeffs = FALSE, keepfolds = FALSE,
keepdataY = TRUE, keepMclassed=FALSE, tol_Xi = 10^(-12), weights, method,
verbose=TRUE)
PLS_glm_kfoldcv_formula(formula,data=NULL,nt=2,limQ2set=.0975,modele="pls",
family=NULL, K=5, NK=1, grouplist=NULL, random=TRUE,
scaleX=TRUE, scaleY=NULL, keepcoeffs=FALSE, keepfolds=FALSE, keepdataY=TRUE,
keepMclassed=FALSE, tol_Xi=10^(-12),weights,subset,start=NULL,etastart,
mustart,offset,method,control= list(),contrasts=NULL, verbose=TRUE)
```

#### **Arguments**

x	a formula or a response (training) dataset
dataY	response (training) dataset
dataX	predictor(s) (training) dataset
formula	an object of class "formula" (or one that can be coerced to that class): a symbolic description of the model to be fitted. The details of model specification are given under 'Details'.

data an optional data frame, list or environment (or object coercible by as. data. frame

to a data frame) containing the variables in the model. If not found in data, the variables are taken from environment (formula), typically the environment

from which plsRglm is called.

nt number of components to be extracted

limQ2set limit value for the Q2

modele name of the PLS glm model to be fitted ("pls", "pls-glm-Gamma", "pls-glm-gaussian",

"pls-glm-inverse.gaussian", "pls-glm-logistic", "pls-glm-poisson", "pls-glm-polr"). Use "modele=pls-glm-family" to enable the family op-

tion.

family a description of the error distribution and link function to be used in the model.

This can be a character string naming a family function, a family function or the result of a call to a family function. (See family for details of family functions.) To use the family option, please set modele="pls-glm-family". User defined

families can also be defined. See details.

K number of groups. Defaults to 5.

NK number of times the group division is made grouplist to specify the members of the K groups

random should the K groups be made randomly. Defaults to TRUE

scaleX scale the predictor(s): must be set to TRUE for modele="pls" and should be

for glms pls.

scaleY scale the response: Yes/No. Ignored since non always possible for glm re-

sponses.

keepcoeffs shall the coefficients for each model be returned keepfolds shall the groups' composition be returned

keepdataY shall the observed value of the response for each one of the predicted value be

returned

keepMclassed shall the number of miss classed be returned (unavailable)

tol\_Xi minimal value for Norm2(Xi) and  $det(pp' \times pp)$  if there is any missing value in

the dataX. It defaults to  $10^{-12}$ 

weights an optional vector of 'prior weights' to be used in the fitting process. Should be

NULL or a numeric vector.

subset an optional vector specifying a subset of observations to be used in the fitting

process.

start starting values for the parameters in the linear predictor.

etastart starting values for the linear predictor.
mustart starting values for the vector of means.

offset this can be used to specify an a priori known component to be included in the

linear predictor during fitting. This should be NULL or a numeric vector of length equal to the number of cases. One or more offset terms can be included in the formula instead or as well, and if more than one is specified their sum is used.

See model.offset.

method for fitting glms with glm ("pls-glm-Gamma", "pls-glm-gaussian", "pls-glm-inverse.gaussian"

the method to be used in fitting the model. The default method "glm.fit" uses iteratively reweighted least squares (IWLS). User-supplied fitting functions can be supplied either as a function or a character string naming a function, with a function which takes the same arguments as glm.fit. If

"model.frame", the model frame is returned.

pls-glm-polr logistic, probit, complementary log-log or cauchit (corresponding to a Cauchy latent variable).

control a list of parameters for controlling the fitting process. For glm. fit this is passed

to glm.control.

contrasts an optional list. See the contrasts.arg of model.matrix.default.

verbose should info messages be displayed?

... arguments to pass to cv.plsRglmmodel.default or to cv.plsRglmmodel.formula

#### **Details**

Predicts 1 group with the K-1 other groups. Leave one out cross validation is thus obtained for K==nrow(dataX).

There are seven different predefined models with predefined link functions available:

"pls" ordinary pls models

"pls-glm-Gamma" glm gaussian with inverse link pls models

"pls-glm-gaussian" glm gaussian with identity link pls models

"pls-glm-inverse-gamma" glm binomial with square inverse link pls models

"pls-glm-logistic" glm binomial with logit link pls models

"pls-glm-poisson" glm poisson with log link pls models

"pls-glm-polr" glm polr with logit link pls models

Using the "family=" option and setting "modele=pls-glm-family" allows changing the family and link function the same way as for the glm function. As a consequence user-specified families can also be used.

The gaussian family accepts the links (as names) identity, log and inverse.

**The** binomial **family** accepts the links logit, probit, cauchit, (corresponding to logistic, normal and Cauchy CDFs respectively) log and cloglog (complementary log-log).

The Gamma family accepts the links inverse, identity and log.

**The** poisson **family** accepts the links log, identity, and sqrt.

The inverse gaussian family accepts the links 1/mu<sup>2</sup>, inverse, identity and log.

**The** quasi **family** accepts the links logit, probit, cloglog, identity, inverse, log, 1/mu<sup>2</sup> and sqrt.

**The function** power can be used to create a power link function.

... arguments to pass to cv.plsRglmmodel.default or to cv.plsRglmmodel.formula

A typical predictor has the form response ~ terms where response is the (numeric) response vector and terms is a series of terms which specifies a linear predictor for response. A terms specification of the form first + second indicates all the terms in first together with all the terms in second with any duplicates removed.

A specification of the form first:second indicates the set of terms obtained by taking the interactions of all terms in first with all terms in second. The specification first\*second indicates the cross of first and second. This is the same as first + second + first:second.

The terms in the formula will be re-ordered so that main effects come first, followed by the interactions, all second-order, all third-order and so on: to avoid this pass a terms object as the formula.

Non-NULL weights can be used to indicate that different observations have different dispersions (with the values in weights being inversely proportional to the dispersions); or equivalently, when the elements of weights are positive integers w\_i, that each response y\_i is the mean of w\_i unit-weight observations.

#### Value

An object of class "cv.plsRglmmodel".

results\_kfolds list of NK. Each element of the list sums up the results for a group division:

list of K matrices of size about nrow(dataX)/K \* nt with the predicted values for a growing number of components

•••

list of K matrices of size about nrow(dataX)/K \* nt with the predicted values for a growing number of components

folds list of NK. Each element of the list sums up the informations for a group division:

list of K vectors of length about nrow(dataX) with the numbers of the rows of dataX that were used as a training set

• • • · · ·

list of K vectors of length about nrow(dataX) with the numbers of the rows of dataX that were used as a training set

dataY\_kfolds list of NK. Each element of the list sums up the results for a group division:

list of K matrices of size about nrow(dataX)/K \* 1 with the observed values of the response

•••

list of K matrices of size about nrow(dataX)/K \* 1 with the observed values of the response

call the call of the function

# Note

Work for complete and incomplete datasets.

#### Author(s)

```
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```

#### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18.

#### See Also

Summary method summary.cv.plsRglmmodel. kfolds2coeff, kfolds2Pressind, kfolds2Press, kfolds2Mclassedind, kfolds2Mclassed and summary to extract and transform results from k-fold cross validation.

```
data(Cornell)
XCornell<-Cornell[,1:7]</pre>
yCornell<-Cornell[,8]
bbb <- cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=10)</pre>
(sum1<-summary(bbb))</pre>
cvtable(sum1)
bbb2 <- cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=3,</pre>
modele="pls-glm-family",family=gaussian(),K=12)
(sum2<-summary(bbb2))</pre>
cvtable(sum2)
#random=TRUE is the default to randomly create folds for repeated CV
bbb3 <- cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=3,</pre>
modele="pls-glm-family",family=gaussian(),K=6,NK=10)
(sum3<-summary(bbb3))</pre>
plot(cvtable(sum3))
data(aze_compl)
Xaze_compl<-aze_compl[,2:34]</pre>
yaze_compl<-aze_compl$y</pre>
bbb <- cv.plsRglm(yaze_compl, Xaze_compl, nt=10, K=10, modele="pls", keepcoeffs=TRUE)
#For Jackknife computations
kfolds2coeff(bbb)
bbb2 <- cv.plsRglm(yaze_compl, Xaze_compl, nt=10, K=10, modele="pls-glm-family",
family=binomial(probit),keepcoeffs=TRUE)
bbb2 <- cv.plsRglm(yaze_compl, Xaze_compl, nt=10, K=10,</pre>
modele="pls-glm-logistic",keepcoeffs=TRUE)
summary(bbb,MClassed=TRUE)
summary(bbb2,MClassed=TRUE)
kfolds2coeff(bbb2)
kfolds2Chisqind(bbb2)
kfolds2Chisq(bbb2)
summary(bbb2)
rm(list=c("Xaze_compl","yaze_compl","bbb","bbb2"))
data(pine)
Xpine<-pine[,1:10]</pre>
ypine<-pine[,11]</pre>
bbb <- cv.plsRglm(dataY=round(ypine),dataX=Xpine,nt=10,modele="pls-glm-family",
family=poisson(log),K=10,keepcoeffs=TRUE,keepfolds=FALSE)
bbb <- cv.plsRglm(dataY=round(ypine),dataX=Xpine,nt=10,</pre>
modele="pls-glm-poisson",K=10,keepcoeffs=TRUE,keepfolds=FALSE)
#For Jackknife computations
kfolds2coeff(bbb)
boxplot(kfolds2coeff(bbb)[,1])
kfolds2Chisqind(bbb)
kfolds2Chisq(bbb)
```

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```
summary(bbb)
PLS_lm(ypine, Xpine, 10, typeVC="standard") $InfCrit
XpineNAX21 <- Xpine</pre>
XpineNAX21[1,2] <- NA
bbb2 <- cv.plsRglm(dataY=round(ypine),dataX=XpineNAX21,nt=10,</pre>
modele="pls-glm-family",family=poisson(log),K=10,keepcoeffs=TRUE,keepfolds=FALSE)
bbb2 <- cv.plsRglm(dataY=round(ypine),dataX=XpineNAX21,nt=10,</pre>
modele="pls-glm-poisson",K=10,keepcoeffs=TRUE,keepfolds=FALSE)
#For Jackknife computations
kfolds2coeff(bbb2)
boxplot(kfolds2coeff(bbb2)[,1])
kfolds2Chisqind(bbb2)
kfolds2Chisq(bbb2)
summary(bbb2)
PLS_lm(ypine, XpineNAX21, 10, typeVC="standard") $InfCrit
rm(list=c("Xpine","XpineNAX21","ypine","bbb","bbb2"))
data(pine)
Xpine<-pine[,1:10]</pre>
ypine<-pine[,11]</pre>
bbb <- cv.plsRglm(dataY=ypine,dataX=Xpine,nt=10,modele="pls-glm-family",</pre>
family=Gamma,K=10,keepcoeffs=TRUE,keepfolds=FALSE)
bbb <- cv.plsRglm(dataY=ypine,dataX=Xpine,nt=10,modele="pls-glm-Gamma",</pre>
K=10,keepcoeffs=TRUE,keepfolds=FALSE)
#For Jackknife computations
kfolds2coeff(bbb)
boxplot(kfolds2coeff(bbb)[,1])
kfolds2Chisqind(bbb)
kfolds2Chisq(bbb)
summary(bbb)
PLS_lm(ypine, Xpine, 10, typeVC="standard") $InfCrit
XpineNAX21 <- Xpine</pre>
XpineNAX21[1,2] <- NA
bbb2 <- cv.plsRglm(dataY=ypine,dataX=XpineNAX21,nt=10,</pre>
modele="pls-glm-family",family=Gamma(),K=10,keepcoeffs=TRUE,keepfolds=FALSE)
bbb2 <- cv.plsRglm(dataY=ypine,dataX=XpineNAX21,nt=10,</pre>
modele="pls-glm-Gamma",K=10,keepcoeffs=TRUE,keepfolds=FALSE)
#For Jackknife computations
kfolds2coeff(bbb2)
boxplot(kfolds2coeff(bbb2)[,1])
kfolds2Chisqind(bbb2)
kfolds2Chisq(bbb2)
summary(bbb2)
PLS_lm(ypine, XpineNAX21, 10, typeVC="standard") $InfCrit
rm(list=c("Xpine","XpineNAX21","ypine","bbb","bbb2"))
```

```
data(Cornell)
XCornell<-Cornell[,1:7]</pre>
yCornell<-Cornell[,8]
bbb <- cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=10,NK=1,modele="pls")</pre>
summary(bbb)
cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=3,modele="pls-glm-inverse.gaussian",K=12)
cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=3,modele="pls-glm-family",
family=inverse.gaussian,K=12)
cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=3,modele="pls-glm-inverse.gaussian",K=6,
NK=2)$results_kfolds
cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=3,modele="pls-glm-family",family=inverse.gaussian(),
K=6,NK=2)$results_kfolds
cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=3,modele="pls-glm-inverse.gaussian",K=6,
NK=2)$results_kfolds
cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=3,modele="pls-glm-family",
family=inverse.gaussian(link = "1/mu^2"),K=6,NK=2)$results_kfolds
bbb2 <- cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=10,</pre>
modele="pls-glm-inverse.gaussian",keepcoeffs=TRUE)
#For Jackknife computations
kfolds2coeff(bbb2)
boxplot(kfolds2coeff(bbb2)[,1])
kfolds2Chisqind(bbb2)
kfolds2Chisq(bbb2)
summary(bbb2)
PLS_lm(yCornell, XCornell, 10, typeVC="standard") $InfCrit
rm(list=c("XCornell","yCornell","bbb","bbb2"))
data(Cornell)
bbb <- cv.plsRglm(Y~.,data=Cornell,nt=10,NK=1,modele="pls")</pre>
summary(bbb)
cv.plsRglm(Y~.,data=Cornell,nt=3,modele="pls-glm-family",family=gaussian(),K=12)
cv.plsRglm(Y^-.,data=Cornell,nt=3,modele="pls-glm-family",family=gaussian(),K=6,
NK=2, random=TRUE, keepfolds=TRUE) $results_kfolds
#Different ways of model specifications
cv.plsRglm(Y~.,data=Cornell,nt=3,modele="pls-glm-family",family=gaussian(),K=6,
NK=2)$results_kfolds
cv.plsRglm(Y~.,data=Cornell,nt=3,modele="pls-glm-family",family=gaussian,
K=6,NK=2)$results_kfolds
cv.plsRglm(Y~.,data=Cornell,nt=3,modele="pls-glm-family",family=gaussian(),
K=6,NK=2)$results_kfolds
\verb|cv.plsRglm(Y^-.,data=Cornell,nt=3,modele="pls-glm-family",family=gaussian(link=log)|,
K=6,NK=2)$results_kfolds
bbb2 <- cv.plsRglm(Y~.,data=Cornell,nt=10,</pre>
modele="pls-glm-gaussian",keepcoeffs=TRUE)
bbb2 <- cv.plsRglm(Y~.,data=Cornell,nt=3,modele="pls-glm-family",
family=gaussian(link=log),K=6,keepcoeffs=TRUE)
#For Jackknife computations
```

```
kfolds2coeff(bbb2)
boxplot(kfolds2coeff(bbb2)[,1])
kfolds2Chisqind(bbb2)
kfolds2Chisq(bbb2)
summary(bbb2)
PLS\_lm\_formula(Y^{\sim}.,data=Cornell,10,typeVC="standard")\\ \$InfCrit
rm(list=c("bbb","bbb2"))
data(pine)
bbb <- cv.plsRglm(x11~.,data=pine,nt=10,modele="pls-glm-family",
family=gaussian(log),K=10,keepcoeffs=TRUE,keepfolds=FALSE)
bbb <- cv.plsRglm(x11~.,data=pine,nt=10,modele="pls-glm-family",family=gaussian(),
K=10,keepcoeffs=TRUE,keepfolds=FALSE)
#For Jackknife computations
kfolds2coeff(bbb)
boxplot(kfolds2coeff(bbb)[,1])
kfolds2Chisqind(bbb)
kfolds2Chisq(bbb)
summary(bbb)
PLS_lm_formula(x11~.,data=pine,nt=10,typeVC="standard")$InfCrit
pineNAX21 <- pine</pre>
pineNAX21[1,2] <- NA</pre>
bbb2 <- cv.plsRglm(x11~.,data=pineNAX21,nt=10,</pre>
modele="pls-glm-family",family=gaussian(log),K=10,keepcoeffs=TRUE,keepfolds=FALSE)
bbb2 <- cv.plsRglm(x11~.,data=pineNAX21,nt=10,
modele="pls-glm-gaussian",K=10,keepcoeffs=TRUE,keepfolds=FALSE)
#For Jackknife computations
kfolds2coeff(bbb2)
boxplot(kfolds2coeff(bbb2)[,1])
kfolds2Chisqind(bbb2)
kfolds2Chisq(bbb2)
summary(bbb2)
PLS_lm_formula(x11~.,data=pineNAX21,nt=10,typeVC="standard")$InfCrit
rm(list=c("pineNAX21","bbb","bbb2"))
data(aze_compl)
bbb <- cv.plsRglm(y~.,data=aze_compl,nt=10,K=10,modele="pls",
keepcoeffs=TRUE)
#For Jackknife computations
kfolds2coeff(bbb)
bbb2 <- cv.plsRglm(y~.,data=aze_compl,nt=3,K=10,
modele="pls-glm-family",family=binomial(probit),keepcoeffs=TRUE)
bbb2 <- cv.plsRglm(y~.,data=aze_compl,nt=3,K=10,</pre>
modele="pls-glm-logistic",keepcoeffs=TRUE)
summary(bbb,MClassed=TRUE)
summary(bbb2,MClassed=TRUE)
kfolds2coeff(bbb2)
```

```
kfolds2Chisqind(bbb2)
kfolds2Chisq(bbb2)
summary(bbb2)
rm(list=c("bbb","bbb2"))
data(pine)
bbb <- cv.plsRglm(round(x11)~.,data=pine,nt=10,</pre>
modele="pls-glm-family",family=poisson(log),K=10,keepcoeffs=TRUE,keepfolds=FALSE)
bbb <- cv.plsRglm(round(x11)~.,data=pine,nt=10,
modele="pls-glm-poisson",K=10,keepcoeffs=TRUE,keepfolds=FALSE)
#For Jackknife computations
kfolds2coeff(bbb)
boxplot(kfolds2coeff(bbb)[,1])
kfolds2Chisqind(bbb)
kfolds2Chisq(bbb)
summary(bbb)
PLS_lm_formula(x11~.,data=pine,10,typeVC="standard")$InfCrit
pineNAX21 <- pine
pineNAX21[1,2] <- NA</pre>
bbb2 <- cv.plsRglm(round(x11)~.,data=pineNAX21,nt=10,</pre>
modele="pls-glm-family",family=poisson(log),K=10,keepcoeffs=TRUE,keepfolds=FALSE)
bbb2 <- cv.plsRglm(round(x11)~.,data=pineNAX21,nt=10,</pre>
modele="pls-glm-poisson",K=10,keepcoeffs=TRUE,keepfolds=FALSE)
#For Jackknife computations
kfolds2coeff(bbb2)
boxplot(kfolds2coeff(bbb2)[,1])
kfolds2Chisqind(bbb2)
kfolds2Chisq(bbb2)
summary(bbb2)
PLS_lm_formula(x11~.,data=pineNAX21,10,typeVC="standard")$InfCrit
rm(list=c("pineNAX21","bbb","bbb2"))
data(pine)
bbb <- cv.plsRglm(x11~.,data=pine,nt=10,modele="pls-glm-family",
family=Gamma,K=10,keepcoeffs=TRUE,keepfolds=FALSE)
bbb <- cv.plsRglm(x11~.,data=pine,nt=10,modele="pls-glm-Gamma",
K=10, keepcoeffs=TRUE, keepfolds=FALSE)
#For Jackknife computations
kfolds2coeff(bbb)
boxplot(kfolds2coeff(bbb)[,1])
kfolds2Chisqind(bbb)
kfolds2Chisq(bbb)
PLS_lm_formula(x11~.,data=pine,10,typeVC="standard")$InfCrit
pineNAX21 <- pine</pre>
```

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```
pineNAX21[1,2] <- NA
bbb2 <- cv.plsRglm(x11~.,data=pineNAX21,nt=10,
modele="pls-glm-family",family=Gamma(),K=10,keepcoeffs=TRUE,keepfolds=FALSE)
bbb2 <- cv.plsRglm(x11~.,data=pineNAX21,nt=10,</pre>
modele="pls-glm-Gamma",K=10,keepcoeffs=TRUE,keepfolds=FALSE)
#For Jackknife computations
kfolds2coeff(bbb2)
boxplot(kfolds2coeff(bbb2)[,1])
kfolds2Chisqind(bbb2)
kfolds2Chisq(bbb2)
summary(bbb2)
PLS_lm_formula(x11~.,data=pineNAX21,10,typeVC="standard")$InfCrit
rm(list=c("pineNAX21","bbb","bbb2"))
data(Cornell)
bbb <- cv.plsRglm(Y~.,data=Cornell,nt=10,NK=1,modele="pls")</pre>
summary(bbb)
cv.plsRglm(Y~.,data=Cornell,nt=3,
modele="pls-glm-inverse.gaussian",K=12)
cv.plsRglm(Y~.,data=Cornell,nt=3,modele="pls-glm-inverse.gaussian",K=6,
NK=2)$results_kfolds
cv.plsRglm(Y~.,data=Cornell,nt=3,modele="pls-glm-family",
family = inverse.gaussian(), K=6, NK=2) \\ $results_k folds
cv.plsRglm(Y~.,data=Cornell,nt=3,modele="pls-glm-inverse.gaussian",K=6,NK=2)$results_kfolds
cv.plsRglm(Y~.,data=Cornell,nt=3,modele="pls-glm-family",
family=inverse.gaussian(link = "1/mu^2"),K=6,NK=2)$results_kfolds
bbb2 <- cv.plsRglm(Y~.,data=Cornell,nt=10,</pre>
modele="pls-glm-inverse.gaussian",keepcoeffs=TRUE)
#For Jackknife computations
kfolds2coeff(bbb2)
boxplot(kfolds2coeff(bbb2)[,1])
kfolds2Chisqind(bbb2)
kfolds2Chisq(bbb2)
summary(bbb2)
PLS_lm_formula(Y~.,data=Cornell,10,typeVC="standard")$InfCrit
rm(list=c("bbb","bbb2"))
data(bordeaux)
bbb <- cv.plsRglm(Quality~.,data=bordeaux,10,</pre>
modele="pls-glm-polr",K=7)
summary(bbb)
bordeauxNA<-bordeaux
bordeauxNA[1,1] <- NA
bbbNA <- cv.plsRglm(Quality~Temperature+Sunshine+Heat+Rain,</pre>
data=bordeauxNA,10,modele="pls-glm-polr",K=10)
summary(bbbNA)
```

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```
rm(list=c("bbb","bbbNA"))
bbb2 <- cv.plsRglm(Quality~.,data=bordeaux,nt=2,K=7,
modele="pls-glm-polr",method="logistic")
bbb3 <- cv.plsRglm(Quality~.,data=bordeaux,nt=2,K=7,
modele="pls-glm-polr",method="probit")
bbb4 <- cv.plsRglm(Quality~.,data=bordeaux,nt=2,K=7,
modele="pls-glm-polr",method="cloglog")
bbb5 <- cv.plsRglm(Quality~.,data=bordeaux,nt=2,K=7,
modele="pls-glm-polr",method="cloglog")
submary(bbb2)
summary(bbb2)
summary(bbb3)
summary(bbb4)
summary(bbb5)
rm(list=c("bbb","bbbNA","bbb2","bbb3","bbb4","bbb5"))</pre>
```

cvtable

Table method for summary of cross validated PLSR and PLSGLR models

## **Description**

The function cvtable is wrapper of cvtable.plsR and cvtable.plsRglm that provides a table summary for the classes "summary.cv.plsRmodel" and "summary.cv.plsRglmmodel"

# Usage

```
cvtable.plsR(x,verbose=TRUE, ...)
cvtable.plsRglm(x,verbose=TRUE, ...)
```

# **Arguments**

```
x an object of the class "summary.cv.plsRmodel"verbose should results be displayed?further arguments to be passed to or from methods.
```

## Value

listList of Information Criteria computed for each fold.

## Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

## References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

40 dicho

#### See Also

```
summary
```

# **Examples**

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
cv.modpls <- cv.plsR(dataY=yCornell,dataX=XCornell,nt=6,K=6,NK=100)
res.cv.modpls <- cvtable(summary(cv.modpls))
plot(res.cv.modpls) #defaults to type="CVQ2"
rm(list=c("XCornell","yCornell","cv.modpls","res.cv.modpls"))

data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
cv.modplsglm <- cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=6,K=6,modele="pls-glm-gaussian",NK=100)
res.cv.modplsglm <- cvtable(summary(cv.modplsglm))
plot(res.cv.modplsglm) #defaults to type="CVQ2Chi2"
rm(list=c("XCornell","yCornell","res.cv.modplsglm"))</pre>
```

dicho

Dichotomization

# Description

This function takes a real value and converts it to 1 if it is positive and else to 0.

# Usage

```
dicho(val)
```

# **Arguments**

val

A real value

#### Value

0 or 1.

## Author(s)

```
Frédéric Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

# See Also

ifelse

fowlkes 41

# **Examples**

```
dimX <- 6
Astar <- 4
(dataAstar4 <- t(replicate(10,simul_data_YX(dimX,Astar))))
dicho(dataAstar4)
rm(list=c("dimX","Astar"))</pre>
```

fowlkes

Fowlkes dataset

# Description

A classic dataset from Fowlkes.

# Usage

```
data(fowlkes)
```

## **Format**

A data frame with 9949 observations on the following 13 variables.

Y binary response

MA a numeric vector

MW a numeric vector

NE a numeric vector

NW a numeric vector

PA a numeric vector

SO a numeric vector

SW a numeric vector

color a numeric vector

age1 a numeric vector

age2 a numeric vector

age3 a numeric vector

sexe a numeric vector

```
data(fowlkes)
str(fowlkes)
```

42 infcrit.dof

infcrit.dof

Information criteria

# **Description**

This function computes information criteria for existing plsR model using Degrees of Freedom estimation.

# Usage

```
infcrit.dof(modplsR, naive = FALSE)
```

## **Arguments**

modplsR A plsR model i.e. an object returned by one of the functions plsR, plsRmodel.default,

plsRmodel.formula, PLS\_lm or PLS\_lm\_formula.

naive A boolean.

#### Details

If naive=FALSE returns AIC, BIC and gmdl values for estimated and naive degrees of freedom. If naive=TRUE returns NULL.

# Value

matrix

AIC, BIC and gmdl values or NULL.

# Author(s)

```
Frederic Bertrand@mat
```

<frederic.bertrand@math.unistra.fr>
http://www-irma.u-strasbg.fr/~fbertran/

#### References

M. Hansen, B. Yu. (2001). Model Selection and Minimum Descripion Length Principle, *Journal of the American Statistical Association*, 96, 746-774.

N. Kraemer, M. Sugiyama. (2011). The Degrees of Freedom of Partial Least Squares Regression. *Journal of the American Statistical Association*, 106(494), 697-705.

N. Kraemer, M. Sugiyama, M.L. Braun. (2009). Lanczos Approximations for the Speedup of Kernel Partial Least Squares Regression, *Proceedings of the Twelfth International Conference on Artificial Intelligence and Statistics (AISTATS)*, 272-279.

# See Also

plsR.dof for degrees of freedom computation and infcrit.dof for computing information criteria directly from a previously fitted plsR model.

kfolds2Chisq 43

## **Examples**

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
modpls <- plsR(yCornell,XCornell,4)
infcrit.dof(modpls)</pre>
```

kfolds2Chisq

Computes Predicted Chisquare for k-fold cross-validated partial least squares regression models.

# Description

This function computes Predicted Chisquare for k-fold cross validated partial least squares regression models.

## Usage

```
kfolds2Chisq(pls_kfolds)
```

# **Arguments**

pls\_kfolds a k-fold cross validated partial least squares regression glm model

## Value

list	Total Predicted Chisquare vs number of components for the first group partition
	•••
list	Total Predicted Chisquare vs number of components for the last group partition

# Note

Use cv.plsRglm to create k-fold cross validated partial least squares regression glm models.

## Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

# References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Francaise de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

## See Also

kfolds2coeff, kfolds2Press, kfolds2Pressind, kfolds2Chisqind, kfolds2Mclassedind and kfolds2Mclassed to extract and transforms results from k-fold cross validation.

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### **Examples**

```
data(Cornell)
XCornell<-Cornell[,1:7]</pre>
yCornell<-Cornell[,8]
bbb <- cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=3,modele="pls-glm-gaussian",K=16)
bbb2 <- cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=3,modele="pls-glm-gaussian",K=5)
kfolds2Chisq(bbb)
kfolds2Chisq(bbb2)
rm(list=c("XCornell","yCornell","bbb","bbb2"))
data(pine)
Xpine<-pine[,1:10]</pre>
ypine<-pine[,11]</pre>
bbb <- cv.plsRglm(dataY=ypine,dataX=Xpine,nt=4,modele="pls-glm-gaussian")</pre>
bbb2 <- cv.plsRglm(dataY=ypine,dataX=Xpine,nt=10,modele="pls-glm-gaussian",K=10)
kfolds2Chisq(bbb)
kfolds2Chisq(bbb2)
XpineNAX21 <- Xpine</pre>
XpineNAX21[1,2] <- NA
bbbNA <- cv.plsRglm(dataY=ypine,dataX=XpineNAX21,nt=10,modele="pls",K=10)</pre>
kfolds2Press(bbbNA)
kfolds2Chisq(bbbNA)
bbbNA2 <- cv.plsRglm(dataY=ypine,dataX=XpineNAX21,nt=4,modele="pls-glm-gaussian")
bbbNA3 <- cv.plsRglm(dataY=ypine,dataX=XpineNAX21,nt=10,modele="pls-glm-gaussian",K=10)
kfolds2Chisq(bbbNA2)
kfolds2Chisq(bbbNA3)
rm(list=c("Xpine","XpineNAX21","ypine","bbb","bbb2","bbbNA","bbbNA2","bbbNA3"))
data(aze_compl)
Xaze_compl<-aze_compl[,2:34]</pre>
yaze_compl<-aze_compl$y</pre>
bbb <- cv.plsRglm(dataY=yaze_compl,dataX=Xaze_compl,nt=4,modele="pls-glm-family",
family="binomial")
bbb <- cv.plsRglm(dataY=yaze_compl,dataX=Xaze_compl,nt=4,modele="pls-glm-logistic")</pre>
bbb2 <- cv.plsRglm(dataY=yaze_compl,dataX=Xaze_compl,nt=10,modele="pls-glm-family",
family=binomial(),K=10)
bbb2 <- cv.plsRglm(dataY=yaze_compl,dataX=Xaze_compl,nt=10,modele="pls-glm-logistic",K=10)
kfolds2Chisq(bbb)
kfolds2Chisq(bbb2)
rm(list=c("Xaze_compl","yaze_compl","bbb","bbb2"))
```

kfolds2Chisqind

Computes individual Predicted Chisquare for k-fold cross validated partial least squares regression models.

# **Description**

This function computes individual Predicted Chisquare for k-fold cross validated partial least squares regression models.

kfolds2Chisqind 45

### Usage

```
kfolds2Chisqind(pls_kfolds)
```

# **Arguments**

pls\_kfolds a k-fold cross validated partial least squares regression glm model

### Value

list Individual PChisq vs number of components for the first group partition
...
list Individual PChisq vs number of components for the last group partition

# Note

Use cv.plsRglm to create k-fold cross validated partial least squares regression glm models.

## Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

#### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

#### See Also

kfolds2coeff, kfolds2Press, kfolds2Pressind, kfolds2Chisq, kfolds2Mclassedind and kfolds2Mclassed to extract and transforms results from k-fold cross-validation.

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
bbb <- cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=3,modele="pls-glm-gaussian",K=16)
bbb2 <- cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=3,modele="pls-glm-gaussian",K=5)
kfolds2Chisqind(bbb)
kfolds2Chisqind(bbb2)
rm(list=c("XCornell","yCornell","bbb","bbb2"))

data(pine)
Xpine<-pine[,1:10]
ypine<-pine[,11]
bbb <- cv.plsRglm(dataY=ypine,dataX=Xpine,nt=4,modele="pls-glm-gaussian")
bbb2 <- cv.plsRglm(dataY=ypine,dataX=Xpine,nt=10,modele="pls-glm-gaussian",K=10)
kfolds2Chisqind(bbb)</pre>
```

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```
kfolds2Chisqind(bbb2)
XpineNAX21 <- Xpine</pre>
XpineNAX21[1,2] <- NA
bbbNA <- cv.plsRglm(dataY=ypine,dataX=XpineNAX21,nt=10,modele="pls",K=10)
kfolds2Pressind(bbbNA)
kfolds2Chisqind(bbbNA)
bbbNA2 <- cv.plsRglm(dataY=ypine,dataX=XpineNAX21,nt=4,modele="pls-glm-gaussian")
bbbNA3 <- cv.plsRglm(dataY=ypine,dataX=XpineNAX21,nt=10,modele="pls-glm-gaussian",K=10)
kfolds2Chisgind(bbbNA2)
kfolds2Chisqind(bbbNA3)
rm(list=c("Xpine","XpineNAX21","ypine","bbb","bbb2","bbbNA","bbbNA2","bbbNA3"))
data(aze_compl)
Xaze_compl<-aze_compl[,2:34]</pre>
yaze_compl<-aze_compl$y</pre>
\verb|bbb| <- cv.plsRglm(dataY=yaze\_compl,dataX=Xaze\_compl,nt=4,modele="pls-glm-family",dataY=yaze\_compl,dataX=Xaze\_compl,nt=4,modele="pls-glm-family",dataY=yaze\_compl,dataX=Xaze\_compl,nt=4,modele="pls-glm-family",dataY=yaze\_compl,dataX=Xaze\_compl,nt=4,modele="pls-glm-family",dataY=yaze\_compl,dataX=Xaze\_compl,nt=4,modele="pls-glm-family",dataY=yaze\_compl,dataX=Xaze\_compl,dataY=yaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xaze\_compl,dataX=Xa
family=binomial())
bbb <- cv.plsRglm(dataY=yaze_compl,dataX=Xaze_compl,nt=4,modele="pls-glm-logistic")
bbb2 <- cv.plsRglm(dataY=yaze_compl,dataX=Xaze_compl,nt=10,modele="pls-glm-family",
family=binomial(),K=10)
bbb2 <- cv.plsRglm(dataY=yaze_compl,dataX=Xaze_compl,nt=10,modele="pls-glm-logistic",K=10)
kfolds2Chisqind(bbb)
kfolds2Chisqind(bbb2)
rm(list=c("Xaze_compl","yaze_compl","bbb","bbb2"))
```

kfolds2coeff

Extracts coefficients from k-fold cross validated partial least squares regression models

#### **Description**

This fonction extracts coefficients from k-fold cross validated partial least squares regression models

# Usage

```
kfolds2coeff(pls_kfolds)
```

## **Arguments**

pls\_kfolds

an object that is a k-fold cross validated partial least squares regression models either lm or glm

# **Details**

This fonctions works for plsR and plsRglm models.

## Value

coef.all

matrix with the values of the coefficients for each leave one out step or NULL if another type of cross validation was used.

kfolds2CVinfos\_glm 47

#### Note

Only for NK=1 and leave one out CV

## Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

## References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

## See Also

kfolds2Pressind, kfolds2Press, kfolds2Mclassedind, kfolds2Mclassed and summary to extract and transform results from k-fold cross validation.

# **Examples**

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
bbb <- PLS_lm_kfoldcv(dataY=yCornell,dataX=XCornell,nt=3,K=nrow(XCornell),keepcoeffs=TRUE)
kfolds2coeff(bbb)
boxplot(kfolds2coeff(bbb)[,2])
rm(list=c("XCornell","yCornell","Xpine","ypine","bbb"))

data(pine)
Xpine<-pine[,1:10]
ypine<-pine[,11]
bbb2 <- cv.plsR(dataY=ypine,dataX=Xpine,nt=4,K=nrow(Xpine),keepcoeffs=TRUE)
kfolds2coeff(bbb2)
boxplot(kfolds2coeff(bbb2)[,1])
rm(list=c("Xpine","ypine","Xpine","ypine","bbb2"))</pre>
```

kfolds2CVinfos\_glm

Extracts and computes information criteria and fits statistics for k-fold cross validated partial least squares glm models

## **Description**

This function extracts and computes information criteria and fits statistics for k-fold cross validated partial least squares glm models for both formula or classic specifications of the model.

# Usage

```
kfolds2CVinfos_glm(pls_kfolds, MClassed = FALSE, verbose=TRUE)
```

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### **Arguments**

pls\_kfolds an object computed using cv.plsRglm

MClassed should number of miss classed be computed?

verbose should infos be displayed?

#### **Details**

The Mclassed option should only set to TRUE if the response is binary.

#### Value

```
list table of fit statistics for first group partition...list table of fit statistics for last group partition
```

#### Note

Use summary and cv.plsRglm instead.

# Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

## References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

#### See Also

kfolds2coeff, kfolds2Pressind, kfolds2Press, kfolds2Mclassedind and kfolds2Mclassed to extract and transforms results from k-fold cross-validation.

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
bbb <- cv.plsRglm(dataY=yCornell,dataX=data.frame(scale(as.matrix(XCornell))[,]),
nt=6,K=12,NK=1,keepfolds=FALSE,keepdataY=TRUE,modele="pls")
summary(bbb,MClassed=TRUE)
rm(list=c("XCornell","yCornell","bbb"))

data(aze_compl)
Xaze_compl<-aze_compl[,2:34]
yaze_compl<-aze_compl$y
bbb <- cv.plsR(yaze_compl,Xaze_compl,nt=10,K=8,modele="pls")</pre>
```

kfolds2Mclassed 49

```
summary(bbb,MClassed=TRUE)
bbbbis <- cv.plsRglm(yaze_compl, Xaze_compl, nt=10, K=8, modele="pls")</pre>
summary(bbbbis,MClassed=TRUE)
bbba <- cv.plsRglm(yaze_compl, Xaze_compl, nt=10, K=8,</pre>
modele="pls-glm-family",family=gaussian())
summary(bbba,MClassed=TRUE)
bbb2 <- cv.plsRglm(yaze_compl, Xaze_compl, nt=10, K=8,</pre>
modele="pls-glm-logistic")
summary(bbb2,MClassed=TRUE)
bbb2a <- cv.plsRglm(yaze_compl, Xaze_compl, nt=10, K=8,
modele="pls-glm-family",family=binomial())
summary(bbb2a,MClassed=TRUE)
rm(list=c("Xaze_compl","yaze_compl","bbb","bbbbis","bbb2","bbb2","bbb2a"))
if(require(chemometrics)){
data(hyptis)
hyptis
yhyptis <- factor(hyptis$Group,ordered=TRUE)</pre>
Xhyptis <- as.data.frame(hyptis[,c(1:6)])</pre>
options(contrasts = c("contr.treatment", "contr.poly"))
modpls2 <- plsRglm(yhyptis, Xhyptis, 6, modele="pls-glm-polr")</pre>
modpls2$Coeffsmodel_vals
modpls2$InfCrit
modpls2$Coeffs
modpls2$std.coeffs
table(yhyptis,predict(modpls2$FinalModel,type="class"))
modpls 3 <- PLS_glm(yhyptis[-c(1,2,3)], Xhyptis[-c(1,2,3),], 3, modele="pls-glm-polr", Algorithm of the context of the conte
dataPredictY=Xhyptis[c(1,2,3),])
bbb <- cv.plsRglm(yhyptis,Xhyptis,nt=4,K=10,random=TRUE,modele="pls-glm-polr",
keepcoeffs=TRUE)
summary(bbb,MClassed=TRUE)
}
```

kfolds2Mclassed

Number of missclassified individuals for k-fold cross validated partial least squares regression models.

## **Description**

This function indicates the total number of missclassified individuals for k-fold cross validated partial least squares regression models.

# Usage

```
kfolds2Mclassed(pls_kfolds)
```

## **Arguments**

pls\_kfolds

a k-fold cross validated partial least squares regression model used on binary data

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#### Value

list	Total number of missclassified individuals vs number of components for the first group partition
• • •	•••
list	Total number of missclassified individuals vs number of components for the last group partition

#### Note

Use cv.plsR to create k-fold cross validated partial least squares regression models.

## Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

#### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

# See Also

k folds 2 Coeff, k folds 2 Press, k folds 2 Pressind and k folds 2 Mclassed ind to extract and transforms results from k-fold cross validation.

## **Examples**

```
data(aze_compl)
Xaze_compl<-aze_compl[,2:34]
yaze_compl<-aze_compl$y
bbb <- cv.plsR(dataY=yaze_compl,dataX=Xaze_compl,nt=10,K=8,NK=1)
bbb2 <- cv.plsR(dataY=yaze_compl,dataX=Xaze_compl,nt=10,K=8,NK=2)
kfolds2Mclassed(bbb)
kfolds2Mclassed(bbb2)
rm(list=c("Xaze_compl","yaze_compl","bbb","bbb2"))</pre>
```

kfolds2Mclassedind

Number of missclassified individuals per group for k-fold cross validated partial least squares regression models.

# **Description**

This function indicates the number of missclassified individuals per group for k-fold cross validated partial least squares regression models.

kfolds2Mclassedind 51

### Usage

```
kfolds2Mclassedind(pls_kfolds)
```

## **Arguments**

pls\_kfolds a k-fold cross validated partial least squares regression model used on binary

data

## Value

Number of missclassified individuals per group vs number of components for the first group partition

...

list Number of missclassified individuals per group vs number of components for

the last group partition

#### Note

Use cv.plsR or cv.plsRglm to create k-fold cross validated partial least squares regression models or generalized linear ones.

## Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

#### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

## See Also

kfolds2coeff, kfolds2Press, kfolds2Pressind and kfolds2Mclassed to extract and transforms results from k-fold cross-validation.

```
data(aze_compl)
Xaze_compl<-aze_compl[,2:34]
yaze_compl<-aze_compl$y
bbb <- cv.plsR(dataY=yaze_compl,dataX=Xaze_compl,nt=10,K=8,NK=1)
bbb2 <- cv.plsR(dataY=yaze_compl,dataX=Xaze_compl,nt=10,K=8,NK=2)
kfolds2Mclassedind(bbb)
kfolds2Mclassedind(bbb2)
rm(list=c("Xaze_compl","yaze_compl","bbb","bbb2"))</pre>
```

52 kfolds2Press

kfolds2Press Computes PRESS for k-fold cross validated partial least squares regression models.	-
---	---

## **Description**

This function computes PRESS for k-fold cross validated partial least squares regression models.

# Usage

```
kfolds2Press(pls_kfolds)
```

## **Arguments**

```
pls_kfolds a k-fold cross validated partial least squares regression model
```

## Value

list	Press vs number of components for the first group partition
	•••
list	Press vs number of components for the last group partition

## Note

Use cv.plsR to create k-fold cross validated partial least squares regression models.

## Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

## References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

## See Also

kfolds2coeff, kfolds2Pressind, kfolds2Mclassedind and kfolds2Mclassed to extract and transforms results from k-fold cross validation.

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
bbb <- cv.plsR(dataY=yCornell,dataX=data.frame(scale(as.matrix(XCornell))[,]),nt=6,K=12,NK=1)
bbb2 <- cv.plsR(dataY=yCornell,dataX=data.frame(scale(as.matrix(XCornell))[,]),nt=6,K=6,NK=1)
kfolds2Press(bbb)</pre>
```

kfolds2Pressind 53

```
kfolds2Press(bbb2)
rm(list=c("XCornell","yCornell","bbb","bbb2"))
data(pine)
Xpine<-pine[,1:10]</pre>
ypine<-pine[,11]</pre>
bbb <- cv.plsR(dataY=ypine,dataX=Xpine,nt=10,NK=1)</pre>
bbb2 <- cv.plsR(dataY=ypine,dataX=Xpine,nt=10,NK=2)</pre>
kfolds2Press(bbb)
kfolds2Press(bbb2)
XpineNAX21 <- Xpine</pre>
XpineNAX21[1,2] <- NA</pre>
bbbNA <- cv.plsR(dataY=ypine,dataX=XpineNAX21,nt=10,NK=1)</pre>
bbbNA2 <- cv.plsR(dataY=ypine,dataX=XpineNAX21,nt=10,NK=2)
kfolds2Press(bbbNA)
kfolds2Press(bbbNA2)
rm(list=c("Xpine","XpineNAX21","ypine","bbb","bbb2","bbbNA","bbbNA2"))
```

kfolds2Pressind

Computes individual PRESS for k-fold cross validated partial least squares regression models.

# **Description**

This function computes individual PRESS for k-fold cross validated partial least squares regression models.

## Usage

```
kfolds2Pressind(pls_kfolds)
```

## **Arguments**

pls\_kfolds a k-fold cross validated partial least squares regression model

# Value

list Individual Press vs number of components for the first group partition
...

list Individual Press vs number of components for the last group partition

## Note

Use cv.plsR to create k-fold cross validated partial least squares regression models.

# Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

54 loglikpls

#### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

## See Also

kfolds2coeff, kfolds2Press, kfolds2Mclassedind and kfolds2Mclassed to extract and transforms results from k-fold cross validation.

## **Examples**

```
data(Cornell)
XCornell<-Cornell[,1:7]</pre>
yCornell<-Cornell[,8]
bbb <- cv.plsR(dataY=yCornell,dataX=data.frame(scale(as.matrix(XCornell))[,]),nt=6,K=12,NK=1)
bbb2 <- cv.plsR(dataY=yCornell,dataX=data.frame(scale(as.matrix(XCornell))[,]),nt=6,K=6,NK=1)\\
kfolds2Pressind(bbb)
kfolds2Pressind(bbb2)
rm(list=c("XCornell","yCornell","bbb","bbb2"))
data(pine)
Xpine<-pine[,1:10]</pre>
ypine<-pine[,11]</pre>
bbb <- cv.plsR(dataY=ypine,dataX=Xpine,nt=10,NK=1)</pre>
bbb2 <- cv.plsR(dataY=ypine,dataX=Xpine,nt=10,NK=2)</pre>
kfolds2Pressind(bbb)
kfolds2Pressind(bbb2)
XpineNAX21 <- Xpine</pre>
XpineNAX21[1,2] <- NA
bbbNA <- cv.plsR(dataY=ypine,dataX=XpineNAX21,nt=10,NK=1)</pre>
bbbNA2 <- cv.plsR(dataY=ypine,dataX=XpineNAX21,nt=10,NK=2)
kfolds2Pressind(bbbNA)
kfolds2Pressind(bbbNA2)
rm(list=c("Xpine","XpineNAX21","ypine","bbb","bbb2","bbbNA","bbbNA2"))
```

loglikpls

loglikelihood function for plsR models

# **Description**

This function provides loglikelihood computation for an univariate plsR model.

# Usage

```
loglikpls(residpls, weights=rep.int(1,length(residpls)))
```

loglikpls 55

## **Arguments**

residpls Residuals of a fitted univariate plsR model

weights Weights of observations

## **Details**

Loglikelihood functions for plsR models with univariate response.

#### Value

real Loglikelihood value

### Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

#### References

Baibing Li, Julian Morris, Elaine B. Martin, Model selection for partial least squares regression, Chemometrics and Intelligent Laboratory Systems 64 (2002) 79-89. http://dx.doi.org/10.1016/S0169-7439(02)00051-5

## See Also

AICpls for AIC computation and logLik for loglikelihood computations for linear models

```
data(pine)
ypine <- pine[,11]</pre>
Xpine <- pine[,1:10]</pre>
(Pinscaled <- as.data.frame(cbind(scale(ypine), scale(as.matrix(Xpine)))))</pre>
colnames(Pinscaled)[1] <- "yy"</pre>
lm(yy^x1+x2+x3+x4+x5+x6+x7+x8+x9+x10, data=Pinscaled)
modpls <- plsR(ypine, Xpine, 10)</pre>
modpls$Std.Coeffs
lm(yy^x1+x2+x3+x4+x5+x6+x7+x8+x9+x10, data=Pinscaled)
AIC(lm(yy^x1+x2+x3+x4+x5+x6+x7+x8+x9+x10, data=Pinscaled))
\label{logLik} \\ \texttt{print}(\log \text{Lik}(\text{lm}(yy^*x1+x2+x3+x4+x5+x6+x7+x8+x9+x10}, \text{data=Pinscaled})))
sum(dnorm(modpls$RepY, modpls$Std.ValsPredictY, sqrt(mean(modpls$residY^2)), log=TRUE))
sum(dnorm(Pinscaled\$yy,fitted(lm(yy^*x1+x2+x3+x4+x5+x6+x7+x8+x9+x10,data=Pinscaled)),
sqrt(mean(residuals(lm(yy^x1+x2+x3+x4+x5+x6+x7+x8+x9+x10,data=Pinscaled))^2)), log=TRUE))
loglikpls(modpls$residY)
loglikpls(residuals(lm(yy^x1+x2+x3+x4+x5+x6+x7+x8+x9+x10,data=Pinscaled)))\\
AICpls(10, residuals(lm(yy~x1+x2+x3+x4+x5+x6+x7+x8+x9+x10, data=Pinscaled)))\\
AICpls(10, modpls$residY)
```

56 permcoefs.plsR

permcoefs.plsR	Coefficients for permutation bootstrap computations of PLSR models
h	

## **Description**

A function passed to boot to perform bootstrap.

# Usage

```
permcoefs.plsR(dataset,ind,nt,modele, maxcoefvalues,ifbootfail,verbose)
```

# **Arguments**

dataset dataset to resample ind indices for resampling

nt number of components to use modele type of modele to use, see plsR

maxcoefvalues maximum values allowed for the estimates of the coefficients to discard those

coming from singular bootstrap samples

ifbootfail value to return if the estimation fails on a bootstrap sample

verbose should info messages be displayed?

# Value

estimates on a bootstrap sample or ifbootfail value if the bootstrap computation fails.

## Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

# See Also

See also bootpls.

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]

# Lazraq-Cleroux PLS (Y,X) bootstrap
# statistic=permcoefs.plsR is the default for (Y,X) permutation resampling of PLSR models.
set.seed(250)
modpls <- plsR(yCornell,XCornell,1)
Cornell.bootYX <- bootpls(modpls, sim="permutation", R=250, statistic=permcoefs.plsR)</pre>
```

permcoefs.plsRgIm 57

permcoefs.plsRglm	Coefficients for permutation bootstrap computations of PLSGLR models
	els

# **Description**

A function passed to boot to perform bootstrap.

# Usage

```
permcoefs.plsRglm(dataset, ind, nt, modele, family=NULL, maxcoefvalues,ifbootfail,verbose)
```

# **Arguments**

dataset dataset to resample

ind indices for resampling

nt number of components to use

modele type of modele to use, see plsRglm

family glm family to use, see plsRglm

maxcoefvalues maximum values allowed for the estimates of the coefficients to discard those coming from singular bootstrap samples

value to return if the estimation fails on a bootstrap sample

verbose should info messages be displayed?

# Value

ifbootfail

estimates on a bootstrap sample or ifbootfail value if the bootstrap computation fails.

## Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

## See Also

See also bootplsglm.

```
data(Cornell)
# (Y,X) bootstrap of a PLSGLR model
# statistic=coefs.plsRglm is the default for (Y,X) bootstrap of a PLSGLR models.
set.seed(250)
modplsglm <- plsRglm(Y~.,data=Cornell,1,modele="pls-glm-family",family=gaussian)
Cornell.bootYX <- bootplsglm(modplsglm, R=250, typeboot="plsmodel",
sim="permutation", statistic=permcoefs.plsRglm)</pre>
```

permcoefs.plsRglmnp	Coefficients for permutation bootstrap computations of PLSGLR mod-
	els

## **Description**

A function passed to boot to perform bootstrap.

## Usage

```
permcoefs.plsRglmnp(dataRepYtt, ind, nt, modele, family=NULL,
maxcoefvalues, wwetoile,ifbootfail)
```

# **Arguments**

dataRepYtt components' coordinates to bootstrap

ind indices for resampling

 $\begin{array}{ll} \text{nt} & \text{number of components to use} \\ \text{modele} & \text{type of modele to use, see } \text{plsRglm} \\ \text{family} & \text{glm family to use, see } \text{plsRglm} \end{array}$ 

maxcoefvalues maximum values allowed for the estimates of the coefficients to discard those

coming from singular bootstrap samples

wwetoile values of the Wstar matrix in the original fit

ifbootfail value to return if the estimation fails on a bootstrap sample

## Value

estimates on a bootstrap sample or ifbootfail value if the bootstrap computation fails.

## Note

```
~~some notes~~
```

# Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

### See Also

See also bootplsglm

```
data(Cornell)
# (Y,X) bootstrap of a PLSGLR model
# statistic=coefs.plsRglm is the default for (Y,X) bootstrap of a PLSGLR models.
set.seed(250)
modplsglm <- plsRglm(Y~.,data=Cornell,1,modele="pls-glm-family",family=gaussian)
Cornell.bootYT <- bootplsglm(modplsglm, R=250, statistic=permcoefs.plsRglmnp)</pre>
```

permcoefs.plsRnp 59

permcoefs.plsRnp Coefficients computation	n for permutation bootstrap
---	-----------------------------

# **Description**

A function passed to boot to perform bootstrap.

## Usage

```
permcoefs.plsRnp(dataRepYtt,ind,nt,modele, maxcoefvalues,wwetoile,ifbootfail)
```

## **Arguments**

dataRepYtt components' coordinates to bootstrap

ind indices for resampling

nt number of components to use
modele type of modele to use, see plsRglm

maxcoefvalues maximum values allowed for the estimates of the coefficients to discard those

coming from singular bootstrap samples

wwetoile values of the Wstar matrix in the original fit

ifbootfail value to return if the estimation fails on a bootstrap sample

## Value

estimates on a bootstrap sample or ifbootfail value if the bootstrap computation fails.

# Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

## See Also

See also bootpls

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]

# Lazraq-Cleroux PLS (Y,X) bootstrap
# statistic=coefs.plsR is the default for (Y,X) resampling of PLSR models.
set.seed(250)
modpls <- plsR(yCornell,XCornell,1)
Cornell.bootYT <- bootpls(modpls, R=250, typeboot="fmodel_np", sim="permutation", statistic=permcoefs.plsRnp)</pre>
```

60 pine

pine Pine dataset

## **Description**

The caterpillar dataset was extracted from a 1973 study on pine processionary caterpillars. It assesses the influence of some forest settlement characteristics on the development of caterpillar colonies. The response variable is the logarithmic transform of the average number of nests of caterpillars per tree in an area of 500 square meters (x11). There are k=10 potentially explanatory variables defined on n=33 areas.

## Usage

data(pine)

#### **Format**

A data frame with 33 observations on the following 11 variables.

- x1 altitude (in meters)
- x2 slope (en degrees)
- x3 number of pines in the area
- x4 height (in meters) of the tree sampled at the center of the area
- x5 diameter (in meters) of the tree sampled at the center of the area
- x6 index of the settlement density
- x7 orientation of the area (from 1 if southbound to 2 otherwise)
- x8 height (in meters) of the dominant tree
- x9 number of vegetation strata
- x10 mix settlement index (from 1 if not mixed to 2 if mixed)
- x11 logarithmic transform of the average number of nests of caterpillars per tree

#### **Details**

These caterpillars got their names from their habit of moving over the ground in incredibly long head-to-tail processions when leaving their nest to create a new colony.

The pine\_sup dataset can be used as a test set to assess model prediction error of a model trained on the pine dataset.

### Source

Tomassone R., Audrain S., Lesquoy-de Turckeim E., Millier C. (1992), "La regression, nouveaux regards sur une ancienne methode statistique", INRA, *Actualites Scientifiques et Agronomiques*, Masson, Paris.

## References

J.-M. Marin, C. Robert. (2007). *Bayesian Core: A Practical Approach to Computational Bayesian Statistics*. Springer, New-York, pages 48-49.

pine\_full 61

### **Examples**

```
data(pine)
str(pine)
```

pine\_full

Complete Pine dataset

## **Description**

This is the complete caterpillar dataset from a 1973 study on pine\_full processionary caterpillars. It assesses the influence of some forest settlement characteristics on the development of caterpillar colonies. The response variable is the logarithmic transform of the average number of nests of caterpillars per tree in an area of 500 square meters (x11). There are k=10 potentially explanatory variables defined on n=55 areas.

## Usage

```
data(pine_full)
```

#### **Format**

A data frame with 55 observations on the following 11 variables.

- x1 altitude (in meters)
- x2 slope (en degrees)
- x3 number of pine\_fulls in the area
- x4 height (in meters) of the tree sampled at the center of the area
- x5 diameter (in meters) of the tree sampled at the center of the area
- x6 index of the settlement density
- x7 orientation of the area (from 1 if southbound to 2 otherwise)
- x8 height (in meters) of the dominant tree
- x9 number of vegetation strata
- x10 mix settlement index (from 1 if not mixed to 2 if mixed)
- x11 logarithmic transform of the average number of nests of caterpillars per tree

#### **Details**

These caterpillars got their names from their habit of moving over the ground in incredibly long head-to-tail processions when leaving their nest to create a new colony.

### Source

Tomassone R., Audrain S., Lesquoy-de Turckeim E., Millier C. (1992), "La regression, nouveaux regards sur une ancienne methode statistique", INRA, *Actualites Scientifiques et Agronomiques*, Masson, Paris.

## References

J.-M. Marin, C. Robert. (2007). *Bayesian Core: A Practical Approach to Computational Bayesian Statistics*. Springer, New-York, pages 48-49.

62 pine\_sup

### **Examples**

```
data(pine_full)
str(pine_full)
```

pine\_sup

Complete Pine dataset

# **Description**

This is a supplementary dataset (used as a test set for the pine dataset) that was extracted from a 1973 study on pine\_sup processionary caterpillars. It assesses the influence of some forest settlement characteristics on the development of caterpillar colonies. The response variable is the logarithmic transform of the average number of nests of caterpillars per tree in an area of 500 square meters (x11). There are k=10 potentially explanatory variables defined on n=22 areas.

## Usage

```
data(pine_sup)
```

#### **Format**

A data frame with 22 observations on the following 11 variables.

- x1 altitude (in meters)
- x2 slope (en degrees)
- x3 number of pine\_sups in the area
- x4 height (in meters) of the tree sampled at the center of the area
- x5 diameter (in meters) of the tree sampled at the center of the area
- x6 index of the settlement density
- x7 orientation of the area (from 1 if southbound to 2 otherwise)
- x8 height (in meters) of the dominant tree
- x9 number of vegetation strata
- x10 mix settlement index (from 1 if not mixed to 2 if mixed)
- x11 logarithmic transform of the average number of nests of caterpillars per tree

#### **Details**

These caterpillars got their names from their habit of moving over the ground in incredibly long head-to-tail processions when leaving their nest to create a new colony.

The pine\_sup dataset can be used as a test set to assess model prediction error of a model trained on the pine dataset.

# Source

Tomassone R., Audrain S., Lesquoy-de Turckeim E., Millier C. (1992), "La regression, nouveaux regards sur une ancienne methode statistique", INRA, *Actualites Scientifiques et Agronomiques*, Masson, Paris.

#### References

J.-M. Marin, C. Robert. (2007). *Bayesian Core: A Practical Approach to Computational Bayesian Statistics*. Springer, New-York, pages 48-49.

# **Examples**

```
data(pine_sup)
str(pine_sup)
```

```
plot.table.summary.cv.plsRglmmodel
```

Plot method for table of summary of cross validated plsRglm models

# Description

This function provides a table method for the class "summary.cv.plsRglmmodel"

# Usage

```
## S3 method for class 'table.summary.cv.plsRglmmodel'
plot(x, type=c("CVMC","CVQ2Chi2","CVPreChi2"), ...)
```

# **Arguments**

```
x an object of the class "table.summary.cv.plsRglmmodel"type the type of cross validation criterion to plot.further arguments to be passed to or from methods.
```

### Value

NULL

### Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

# References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

# See Also

summary

### **Examples**

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
bbb <- cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=10,NK=1,
modele="pls-glm-family",family=gaussian())
plot(cvtable(summary(bbb)),type="CVQ2Chi2")
rm(list=c("XCornell","yCornell","bbb"))</pre>
```

```
plot.table.summary.cv.plsRmodel
```

Plot method for table of summary of cross validated plsR models

# **Description**

This function provides a table method for the class "summary.cv.plsRmodel"

# Usage

```
## S3 method for class 'table.summary.cv.plsRmodel'
plot(x, type=c("CVMC","CVQ2","CVPress"), ...)
```

# **Arguments**

```
x an object of the class "table.summary.cv.plsRmodel"type the type of cross validation criterion to plot.further arguments to be passed to or from methods.
```

## Value

NULL

# Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

# References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Francaise de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

# See Also

summary

plots.confints.bootpls 65

## **Examples**

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
bbb <- cv.plsR(dataY=yCornell,dataX=XCornell,nt=6,K=6,NK=100)
plot(cvtable(summary(bbb)),type="CVQ2")
rm(list=c("XCornell","yCornell","bbb"))</pre>
```

```
plots.confints.bootpls
```

Plot bootstrap confidence intervals

# **Description**

This function plots the confidence intervals derived using the function confints.bootpls from from a bootpls based object.

## Usage

```
plots.confints.bootpls(ic_bootobject, indices = NULL, legendpos = "topleft",
prednames = TRUE, articlestyle = TRUE, xaxisticks=TRUE, ltyIC=c(2, 4, 5, 1),
colIC=c("darkgreen", "blue", "red", "black"), typeIC, las = par("las"),
mar, mgp, ...)
```

ic\_bootobject an object created with the confints.bootpls function.

default is c(5, 4, 4, 2) + 0.1.

further options to pass to the plot function.

# **Arguments**

mgp

10_500 005 500	an object created with the committee the factorial
indices	vector of indices of the variables to plot. Defaults to NULL: all the predictors will be used.
legendpos	position of the legend as in legend, defaults to "topleft".
prednames	do the original names of the predictors shall be plotted? Defaults to TRUE: the names are plotted.
articlestyle	do the extra blank zones of the margin shall be removed from the plot? Defaults to TRUE: the margins are removed.
xaxisticks	do ticks for the x axis shall be plotted? Defaults to TRUE: the ticks are plotted.
ltyIC	lty as in plot
colIC	col as in plot
typeIC	type of CI to plot. Defaults to typeIC=c("Normal", "Basic", "Percentile", "BCa") if BCa intervals limits were computed and to typeIC=c("Normal", "Basic", "Percentile") otherwise.
las	numeric in 0,1,2,3; the style of axis labels. 0: always parallel to the axis [default], 1: always horizontal, 2: always perpendicular to the axis, 3: always vertical.
mar	A numerical vector of the form c(bottom, left, top, right) which gives the number of lines of margin to be specified on the four sides of the plot. The

The margin line (in mex units) for the axis title, axis labels and axis line. Note

that mgp[1] affects title whereas mgp[2:3] affect axis. The default is c(3, 1, 0).

#### Value

NULL

## Author(s)

```
Frederic Bertrand
<frederic.bertrand@math.unistra.fr>
http://www-irma.u-strasbg.fr/~fbertran/
```

#### See Also

```
confints.bootpls
```

```
data(Cornell)
modpls <- plsR(Y~.,data=Cornell,3)</pre>
# Lazraq-Cleroux PLS (Y,X) bootstrap
set.seed(250)
Cornell.bootYX <- bootpls(modpls, R=250)</pre>
temp.ci <- confints.bootpls(Cornell.bootYX,2:8)</pre>
plots.confints.bootpls(temp.ci)
plots.confints.bootpls(temp.ci,prednames=FALSE)
\verb|plots.confints.bootpls(temp.ci,prednames=FALSE,articlestyle=FALSE,\\
main="Bootstrap confidence intervals for the bj")
plots.confints.bootpls(temp.ci,indices=1:3,prednames=FALSE)
plots.confints.bootpls(temp.ci,c(2,4,6),"bottomright")
plots.confints.bootpls(temp.ci,c(2,4,6),articlestyle=FALSE,
main="Bootstrap confidence intervals for some of the bj")
temp.ci <- confints.bootpls(Cornell.bootYX,typeBCa=FALSE)</pre>
plots.confints.bootpls(temp.ci)
plots.confints.bootpls(temp.ci,2:8)
plots.confints.bootpls(temp.ci,prednames=FALSE)
# Bastien CSDA 2005 (Y,T) bootstrap
Cornell.boot <- bootpls(modpls, typeboot="fmodel_np", R=250)</pre>
temp.ci <- confints.bootpls(Cornell.boot,2:8)</pre>
plots.confints.bootpls(temp.ci)
plots.confints.bootpls(temp.ci,prednames=FALSE)
plots.confints.bootpls(temp.ci,prednames=FALSE,articlestyle=FALSE,
main="Bootstrap confidence intervals for the bj")
plots.confints.bootpls(temp.ci,indices=1:3,prednames=FALSE)
plots.confints.bootpls(temp.ci,c(2,4,6),"bottomright")
plots.confints.bootpls(temp.ci,c(2,4,6),articlestyle=FALSE,
main="Bootstrap confidence intervals for some of the bj")
temp.ci <- confints.bootpls(Cornell.boot,typeBCa=FALSE)</pre>
plots.confints.bootpls(temp.ci)
plots.confints.bootpls(temp.ci,2:8)
plots.confints.bootpls(temp.ci,prednames=FALSE)
```

```
data(aze_compl)
modplsglm <- plsRglm(y~.,data=aze_compl,3,modele="pls-glm-logistic")</pre>
# Lazraq-Cleroux PLS (Y,X) bootstrap
# should be run with R=1000 but takes much longer time
aze_compl.bootYX3 <- bootplsglm(modplsglm, typeboot="plsmodel", R=250)</pre>
temp.ci <- confints.bootpls(aze_compl.bootYX3)</pre>
plots.confints.bootpls(temp.ci)
plots.confints.bootpls(temp.ci,prednames=FALSE)
plots.confints.bootpls(temp.ci,prednames=FALSE,articlestyle=FALSE,
main="Bootstrap confidence intervals for the bj")
plots.confints.bootpls(temp.ci,indices=1:33,prednames=FALSE)
plots.confints.bootpls(temp.ci,c(2,4,6),"bottomleft")
plots.confints.bootpls(temp.ci,c(2,4,6),articlestyle=FALSE,
main="Bootstrap confidence intervals for some of the bj")
plots.confints.bootpls(temp.ci,indices=1:34,prednames=FALSE)
plots.confints.bootpls(temp.ci,indices=1:33,prednames=FALSE,ltyIC=1,colIC=c(1,2))
temp.ci <- confints.bootpls(aze_compl.bootYX3,1:34,typeBCa=FALSE)</pre>
plots.confints.bootpls(temp.ci,indices=1:33,prednames=FALSE)
# Bastien CSDA 2005 (Y,T) Bootstrap
# much faster
aze_compl.bootYT3 <- bootplsglm(modplsglm, R=1000)</pre>
temp.ci <- confints.bootpls(aze_compl.bootYT3)</pre>
plots.confints.bootpls(temp.ci)
plots.confints.bootpls(temp.ci,typeIC="Normal")
plots.confints.bootpls(temp.ci,typeIC=c("Normal","Basic"))
plots.confints.bootpls(temp.ci,typeIC="BCa",legendpos="bottomleft")
plots.confints.bootpls(temp.ci,prednames=FALSE)
plots.confints.bootpls(temp.ci,prednames=FALSE,articlestyle=FALSE,
main="Bootstrap confidence intervals for the bj")
plots.confints.bootpls(temp.ci,indices=1:33,prednames=FALSE)
plots.confints.bootpls(temp.ci,c(2,4,6),"bottomleft")
plots.confints.bootpls(temp.ci,c(2,4,6),articlestyle=FALSE,
main="Bootstrap confidence intervals for some of the bj")
plots.confints.bootpls(temp.ci,prednames=FALSE,ltyIC=c(2,1),colIC=c(1,2))
temp.ci <- confints.bootpls(aze_compl.bootYT3,1:33,typeBCa=FALSE)</pre>
plots.confints.bootpls(temp.ci,prednames=FALSE)
```

plsR

Partial least squares Regression models with leave one out cross validation

## **Description**

This function implements Partial least squares Regression models with leave one out cross validation for complete or incomplete datasets.

### Usage

```
plsR(x, ...)
## Default S3 method:
plsRmodel(dataY, dataX, nt = 2, limQ2set = 0.0975,
dataPredictY = dataX, modele = "pls", family = NULL, typeVC = "none",
EstimXNA = FALSE, scaleX = TRUE, scaleY = NULL, pvals.expli = FALSE,
alpha.pvals.expli = 0.05, MClassed = FALSE, tol_Xi = 10^(-12), weights,
sparse = FALSE, sparseStop = TRUE, naive = FALSE, verbose=TRUE)
## S3 method for class 'formula'
plsRmodel(formula, data, nt = 2, limQ2set = 0.0975,
dataPredictY, modele = "pls", family = NULL, typeVC = "none",
EstimXNA = FALSE, scaleX = TRUE, scaleY = NULL, pvals.expli = FALSE,
alpha.pvals.expli = 0.05, MClassed = FALSE, tol_Xi = 10^(-12), weights,
subset, contrasts = NULL, sparse = FALSE, sparseStop = TRUE, naive = FALSE,
verbose=TRUE)
PLS_lm(dataY, dataX, nt = 2, limQ2set = 0.0975, dataPredictY = dataX,
modele = "pls", family = NULL, typeVC = "none", EstimXNA = FALSE,
scaleX = TRUE, scaleY = NULL, pvals.expli = FALSE,
alpha.pvals.expli = 0.05, MClassed = FALSE, tol_Xi = 10^(-12),
weights,sparse=FALSE,sparseStop=FALSE,naive=FALSE,verbose=TRUE)
PLS_lm_formula(formula,data=NULL,nt=2,limQ2set=.0975,dataPredictY=dataX,
modele="pls",family=NULL,typeVC="none",EstimXNA=FALSE,scaleX=TRUE,
scaleY=NULL,pvals.expli=FALSE,alpha.pvals.expli=.05,MClassed=FALSE,
tol_Xi=10^(-12),weights,subset,contrasts=NULL,sparse=FALSE,
sparseStop=FALSE,naive=FALSE,verbose=TRUE)
```

# Arguments

x a formula or a response (training) dataset

dataY response (training) dataset dataX predictor(s) (training) dataset

formula an object of class "formula" (or one that can be coerced to that class): a sym-

bolic description of the model to be fitted. The details of model specification are

given under 'Details'.

data an optional data frame, list or environment (or object coercible by as.data.frame

to a data frame) containing the variables in the model. If not found in data, the variables are taken from environment (formula), typically the environment

from which plsR is called.

nt number of components to be extracted

limQ2set limit value for the Q2 dataPredictY predictor(s) (testing) dataset

modele name of the PLS model to be fitted, only ("pls" available for this fonction.

family for the present moment the family argument is ignored and set thanks to the

value of modele.

type of leave one out cross validation. Several procedures are available. If cross

validation is required, one needs to selects the way of predicting the response for left out observations. For complete rows, without any missing value, there are two different ways of computing these predictions. As a consequence, for mixed datasets, with complete and incomplete rows, there are two ways of computing prediction: either predicts any row as if there were missing values in it

(missingdata) or selects the prediction method accordingly to the completeness of the row (adaptative).

none no cross validation

standard as in SIMCA for datasets without any missing value. For datasets with any missing value, it is the as using missing data

missingdata all values predicted as those with missing values for datasets with any missing values

adaptative predict a response value for an x with any missing value as those with missing values and for an x without any missing value as those without missing values.

 $scale \ \ scale \ the \ predictor(s): \ must \ be \ set \ to \ TRUE \ for \ modele="pls" \ and \ should \ be$ 

for glms pls.

scaleY scale the response: Yes/No. Ignored since non always possible for glm re-

sponses.

pvals.expli should individual p-values be reported to tune model selection?

alpha.pvals.expli

level of significance for predictors when pvals.expli=TRUE

MClassed number of missclassified cases, should only be used for binary responses

tol\_Xi minimal value for Norm2(Xi) and  $det(pp' \times pp)$  if there is any missing value in

the dataX. It defaults to  $10^{-12}$ 

weights an optional vector of 'prior weights' to be used in the fitting process. Should be

NULL or a numeric vector.

subset an optional vector specifying a subset of observations to be used in the fitting

process.

contrasts an optional list. See the contrasts.arg of model.matrix.default.

sparse should the coefficients of non-significant predictors (<alpha.pvals.expli) be

set to 0

 $sparse Stop \qquad should component extraction stop when no significant predictors (\verb|<alpha.pvals.expli|)$ 

are found

naive Use the naive estimates for the Degrees of Freedom in plsR? Default is FALSE.

verbose should info messages be displayed?

... arguments to pass to plsRmodel.default or to plsRmodel.formula

### **Details**

There are several ways to deal with missing values that leads to different computations of leave one out cross validation criteria.

A typical predictor has the form response ~ terms where response is the (numeric) response vector and terms is a series of terms which specifies a linear predictor for response. A terms specification of the form first + second indicates all the terms in first together with all the terms in second with any duplicates removed.

A specification of the form first:second indicates the set of terms obtained by taking the interactions of all terms in first with all terms in second. The specification first\*second indicates the cross of first and second. This is the same as first + second + first:second.

The terms in the formula will be re-ordered so that main effects come first, followed by the interactions, all second-order, all third-order and so on: to avoid this pass a terms object as the formula.

Non-NULL weights can be used to indicate that different observations have different dispersions (with the values in weights being inversely proportional to the dispersions); or equivalently, when the elements of weights are positive integers w\_i, that each response y\_i is the mean of w\_i unit-weight observations.

The default estimator for Degrees of Freedom is the Kramer and Sugiyama's one. Information criteria are computed accordingly to these estimations. Naive Degrees of Freedom and Information Criteria are also provided for comparison purposes. For more details, see N. Kraemer and M. Sugiyama. (2011). The Degrees of Freedom of Partial Least Squares Regression. *Journal of the American Statistical Association*, 106(494), 697-705, 2011.

#### Value

nr Number of observations nc Number of predictors

nt Number of requested components
ww raw weights (before L2-normalization)

wwnorm L2 normed weights (to be used with deflated matrices of predictor variables)
wwetoile modified weights (to be used with original matrix of predictor variables)

tt PLS components

pp loadings of the predictor variables

CoeffC coefficients of the PLS components

uscores scores of the response variable

YChapeau predicted response values for the dataX set

residYChapeau residuals of the deflated response on the standardized scale

RepY scaled response vector

na.miss.Y is there any NA value in the response vector YNA indicatrix vector of missing values in RepY

residY deflated scaled response vector ExpliX scaled matrix of predictors

na.miss.X is there any NA value in the predictor matrix XXNA indicator of non-NA values in the predictor matrix

residXX deflated predictor matrix

PredictY response values with NA replaced with 0

press.ind individual PRESS value for each observation (scaled scale)
press.tot total PRESS value for all observations (scaled scale)

family glm family used to fit PLSGLR model

ttPredictY PLS components for the dataset on which prediction was requested

typeVC type of leave one out cross-validation used

dataX predictor values dataY response values

computed\_nt number of components that were computed

CoeffCFull matrix of the coefficients of the predictors

CoeffConstante value of the intercept (scaled scale)

Std. Coeffs Vector of standardized regression coefficients

press.ind2 individual PRESS value for each observation (original scale)

RSSresidY residual sum of squares (scaled scale)

Coeffs Vector of regression coefficients (used with the original data scale)

Yresidus residuals of the PLS model

RSS residual sum of squares (original scale)

residusY residuals of the deflated response on the standardized scale

AIC.std AIC.std vs number of components (AIC computed for the standardized model

AIC AIC vs number of components

optional If the response is assumed to be binary:

i.e. MClassed=TRUE.

MissClassed Number of miss classed results

Probs "Probability" predicted by the model. These are not true probabilities

since they may lay outside of [0,1]

Probs.trc Probability predicted by the model and constrained to belong to

[0,1]

tt Predict Fitted Missing Y

Description of 'comp2'

optional If cross validation was requested:

i.e. typeVC="standard", typeVC="missingdata" or typeVC="adaptative".

R2residY R2 coefficient value on the standardized scale

R2 R2 coefficient value on the original scale

press.tot2 total PRESS value for all observations (original scale)

Q2 Q2 value (standardized scale) limQ2 limit of the Q2 value Q2\_2 Q2 value (original scale)

Q2cum cumulated Q2 (standardized scale)
Q2cum\_2 cumulated Q2 (original scale)

InfCrit table of Information Criteria

Std.ValsPredictY

predicted response values for supplementary dataset (standardized scale)

ValsPredictY predicted response values for supplementary dataset (original scale)

Std. XChapeau estimated values for missing values in the predictor matrix (standardized scale)

XXwotNA predictor matrix with missing values replaced with 0

## Note

Use cv.plsR to cross-validate the plsRglm models and bootpls to bootstrap them.

## Author(s)

Frederic Bertrand

<frederic.bertrand@math.unistra.fr>
http://www-irma.u-strasbg.fr/~fbertran/

#### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

#### See Also

See also plsRglm to fit PLSGLR models.

```
data(Cornell)
XCornell<-Cornell[,1:7]</pre>
yCornell<-Cornell[,8]
#maximum 6 components could be extracted from this dataset
#trying 10 to trigger automatic stopping criterion
modpls10<-plsR(yCornell,XCornell,10)</pre>
modpls10
#With iterative leave one out CV PRESS
modpls6cv<-plsR(yCornell, XCornell, 6, typeVC="standard")</pre>
cv.modpls<-cv.plsR(yCornell, XCornell, 6, NK=100)</pre>
res.cv.modpls<-cvtable(summary(cv.modpls))</pre>
plot(res.cv.modpls)
rm(list=c("XCornell","yCornell","modpls10","modpls6cv"))
#A binary response example
data(aze_compl)
Xaze_compl<-aze_compl[,2:34]</pre>
yaze_compl<-aze_compl$y</pre>
modpls.aze <- plsR(yaze_compl, Xaze_compl, 10, MClassed=TRUE, typeVC="standard")</pre>
modpls.aze
#Direct access to not cross validated values
modpls.aze$AIC
modpls.aze$AIC.std
modpls.aze$MissClassed
#Raw predicted values (not really probabily since not constrained in [0,1]
modpls.aze$Probs
#Truncated to [0;1] predicted values (true probabilities)
modpls.aze$Probs.trc
modpls.aze$Probs-modpls.aze$Probs.trc
#Repeated cross validation of the model (NK=100 times)
cv.modpls.aze<-cv.plsR(yaze_compl,Xaze_compl,10,NK=100)</pre>
res.cv.modpls.aze<-cvtable(summary(cv.modpls.aze,MClassed=TRUE))</pre>
#High discrepancy in the number of component choice using repeated cross validation
#and missclassed criterion
plot(res.cv.modpls.aze)
```

plsR.dof 73

```
rm(list=c("Xaze_compl","yaze_compl","modpls.aze","cv.modpls.aze","res.cv.modpls.aze"))
#24 predictors
dimX < -24
#2 components
Astar <- 2
simul_data_UniYX(dimX,Astar)
dataAstar2 <- t(replicate(250,simul_data_UniYX(dimX,Astar)))</pre>
ydataAstar2 <- dataAstar2[,1]</pre>
XdataAstar2 <- dataAstar2[,2:(dimX+1)]</pre>
modpls.A2<- plsR(ydataAstar2, XdataAstar2, 10, typeVC="standard")</pre>
cv.modpls.A2<-cv.plsR(ydataAstar2,XdataAstar2,10,NK=100)
res.cv.modpls.A2<-cvtable(summary(cv.modpls.A2))</pre>
#Perfect choice for the Q2 criterion in PLSR
plot(res.cv.modpls.A2)
#Binarized response
ysimbin1 <- dicho(ydataAstar2)</pre>
#Binarized predictors
Xsimbin1 <- dicho(XdataAstar2)</pre>
modpls.B2 <- plsR(ysimbin1,Xsimbin1,10,typeVC="standard",MClassed=TRUE)</pre>
modpls.B2
modpls.B2$Probs
modpls.B2$Probs.trc
modpls.B2$MissClassed
plsR(ysimbin1, XdataAstar2, 10, typeVC="standard", MClassed=TRUE) $InfCrit
cv.modpls.B2<-cv.plsR(ysimbin1,Xsimbin1,2,NK=100)</pre>
res.cv.modpls.B2<-cvtable(summary(cv.modpls.B2,MClassed=TRUE))</pre>
#Only one component found by repeated CV missclassed criterion
plot(res.cv.modpls.B2)
rm(list=c("dimX", "Astar", "dataAstar2", "XdataAstar2", "ydataAstar2", "modpls.A2", "cv.modpls.A2",
"res.cv.modpls.A2","Xsimbin1","ysimbin1","modpls.B2","cv.modpls.B2","res.cv.modpls.B2"))
```

plsR.dof

Computation of the Degrees of Freedom

# **Description**

This function computes the Degrees of Freedom using the Krylov representation of PLS and other quantities that are used to get information criteria values. For the time present, it only works with complete datasets.

### Usage

```
plsR.dof(modplsR, naive = FALSE)
```

# **Arguments**

modplsR A plsR model i.e. an object returned by one of the functions plsR, plsRmodel.default,

plsRmodel.formula, PLS\_lm or PLS\_lm\_formula.

naive A boolean.

#### **Details**

If naive=FALSE returns values for estimated degrees of freedom and error dispersion. If naive=TRUE returns returns values for naive degrees of freedom and error dispersion. The original code from Nicole Kraemer and Mikio L. Braun was unable to handle models with only one component.

#### Value

DoF Degrees of Freedom
sigmahat Estimates of dispersion
Yhat Predicted values

yhat Square Euclidean norms of the predicted values

RSS Residual Sums of Squares

### Author(s)

```
Nicole Kraemer, Mikio L. Braun with improvements from Frederic Bertrand <frederic.bertrand@math.unistra.fr>
http://www-irma.u-strasbg.fr/~fbertran/
```

#### References

N. Kraemer, M. Sugiyama. (2011). The Degrees of Freedom of Partial Least Squares Regression. *Journal of the American Statistical Association*, 106(494), 697-705.

N. Kraemer, M. Sugiyama, M.L. Braun. (2009). Lanczos Approximations for the Speedup of Kernel Partial Least Squares Regression, *Proceedings of the Twelfth International Conference on Artificial Intelligence and Statistics (AISTATS)*, 272-279.

#### See Also

aic.dof and infcrit.dof for computing information criteria directly from a previously fitted plsR model.

# **Examples**

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
modpls <- plsR(yCornell,XCornell,4)
plsR.dof(modpls)
plsR.dof(modpls,naive=TRUE)</pre>
```

plsRglm

Partial least squares Regression generalized linear models

# Description

This function implements Partial least squares Regression generalized linear models complete or incomplete datasets.

#### Usage

```
plsRglm(x, ...)
## Default S3 method:
plsRglmmodel(dataY,dataX,nt=2,limQ2set=.0975,
dataPredictY=dataX,modele="pls",family=NULL,typeVC="none",
EstimXNA=FALSE, scaleX=TRUE, scaleY=NULL, pvals.expli=FALSE,
alpha.pvals.expli=.05,MClassed=FALSE,tol_Xi=10^(-12),weights,
sparse=FALSE, sparseStop=TRUE, naive=FALSE, verbose=TRUE)
## S3 method for class 'formula'
plsRglmmodel(formula,data=NULL,nt=2,limQ2set=.0975,
dataPredictY, modele="pls", family=NULL, typeVC="none",
EstimXNA=FALSE, scaleX=TRUE, scaleY=NULL, pvals.expli=FALSE,
alpha.pvals.expli=.05, \\ MClassed=FALSE, tol\_Xi=10^{-12}, \\ weights, subset,
start=NULL,etastart,mustart,offset,method="glm.fit",control= list(),
contrasts=NULL, sparse=FALSE, sparseStop=TRUE, naive=FALSE, verbose=TRUE)
PLS_glm(dataY, dataX, nt = 2, limQ2set = 0.0975, dataPredictY = dataX,
modele = "pls", family = NULL, typeVC = "none", EstimXNA = FALSE,
scaleX = TRUE, scaleY = NULL, pvals.expli = FALSE,
alpha.pvals.expli = 0.05, MClassed = FALSE, tol_Xi = 10^(-12), weights,
method, sparse = FALSE, sparseStop=FALSE, naive=FALSE, verbose=TRUE)
PLS_glm_formula(formula,data=NULL,nt=2,limQ2set=.0975,dataPredictY=dataX,
modele="pls",family=NULL,typeVC="none",EstimXNA=FALSE,scaleX=TRUE,
scaleY=NULL, pvals.expli=FALSE, alpha.pvals.expli=.05, MClassed=FALSE,
tol_Xi=10^(-12),weights,subset,start=NULL,etastart,mustart,offset,method,
control= list(),contrasts=NULL,sparse=FALSE,sparseStop=FALSE,naive=FALSE,verbose=TRUE)
```

# Arguments

x a formula or a response (training) dataset

dataY response (training) dataset dataX predictor(s) (training) dataset

formula an object of class "formula" (or one that can be coerced to that class): a sym-

bolic description of the model to be fitted. The details of model specification are

given under 'Details'.

data an optional data frame, list or environment (or object coercible by as.data.frame

to a data frame) containing the variables in the model. If not found in data, the variables are taken from environment(formula), typically the environment

from which plsRglm is called.

nt number of components to be extracted

limQ2set limit value for the Q2 dataPredictY predictor(s) (testing) dataset

modele name of the PLS glm model to be fitted ("pls", "pls-glm-Gamma", "pls-glm-gaussian",

"pls-glm-inverse.gaussian", "pls-glm-logistic", "pls-glm-poisson", "pls-glm-polr"). Use "modele=pls-glm-family" to enable the family op-

tion.

family a description of the error distribution and link function to be used in the model.

This can be a character string naming a family function, a family function or the result of a call to a family function. (See family for details of family functions.) To use the family option, please set modele="pls-glm-family". User defined

families can also be defined. See details.

type VC type of leave one out cross validation. For back compatibility purpose.

none no cross validation

EstimXNA only for modele="pls". Set whether the missing X values have to be estimated.

scaleX scale the predictor(s): must be set to TRUE for modele="pls" and should be

for glms pls.

scaleY scale the response: Yes/No. Ignored since non always possible for glm re-

sponses.

pvals.expli should individual p-values be reported to tune model selection?

alpha.pvals.expli

level of significance for predictors when pvals.expli=TRUE

MClassed number of missclassified cases, should only be used for binary responses

tol\_Xi minimal value for Norm2(Xi) and  $det(pp' \times pp)$  if there is any missing value in

the dataX. It defaults to  $10^{-12}$ 

weights an optional vector of 'prior weights' to be used in the fitting process. Should be

NULL or a numeric vector.

subset an optional vector specifying a subset of observations to be used in the fitting

process.

start starting values for the parameters in the linear predictor.

etastart starting values for the linear predictor.

mustart starting values for the vector of means.

offset this can be used to specify an *a priori* known component to be included in the

linear predictor during fitting. This should be NULL or a numeric vector of length equal to the number of cases. One or more offset terms can be included in the formula instead or as well, and if more than one is specified their sum is used.

 $See \ {\tt model.offset}.$ 

method For a glm model (modele="pls-glm-family"), the method to be used in fit-

ting the model. The default method "glm.fit" uses iteratively reweighted least squares (IWLS). User-supplied fitting functions can be supplied either as a function or a character string naming a function, with a function which takes the same arguments as glm.fit. For a polr model (modele="pls-glm-polr"), logistic or probit or (complementary) log-log (loglog or cloglog) or cauchit (corre-

sponding to a Cauchy latent variable).

control a list of parameters for controlling the fitting process. For glm. fit this is passed

to glm.control.

contrasts an optional list. See the contrasts.arg of model.matrix.default.

sparse should the coefficients of non-significant predictors (<alpha.pvals.expli) be

set to 0

sparseStop should component extraction stop when no significant predictors (<alpha.pvals.expli)

are found

naive Use the naive estimates for the Degrees of Freedom in plsR? Default is FALSE.

verbose Should details be displayed?

... arguments to pass to plsRmodel.default or to plsRmodel.formula

#### **Details**

There are seven different predefined models with predefined link functions available:

"pls" ordinary pls models

"pls-glm-Gamma" glm gaussian with inverse link pls models

"pls-glm-gaussian" glm gaussian with identity link pls models

"pls-glm-inverse-gamma" glm binomial with square inverse link pls models

"pls-glm-logistic" glm binomial with logit link pls models

"pls-glm-poisson" glm poisson with log link pls models

"pls-glm-polr" glm polr with logit link pls models

Using the "family=" option and setting "modele=pls-glm-family" allows changing the family and link function the same way as for the glm function. As a consequence user-specified families can also be used.

The gaussian family accepts the links (as names) identity, log and inverse.

**The** binomial **family** accepts the links logit, probit, cauchit, (corresponding to logistic, normal and Cauchy CDFs respectively) log and cloglog (complementary log-log).

The Gamma family accepts the links inverse, identity and log.

The poisson family accepts the links log, identity, and sqrt.

The inverse gaussian family accepts the links 1/mu^2, inverse, identity and log.

**The** quasi **family** accepts the links logit, probit, cloglog, identity, inverse, log, 1/mu<sup>2</sup> and sqrt.

**The function** power can be used to create a power link function.

A typical predictor has the form response ~ terms where response is the (numeric) response vector and terms is a series of terms which specifies a linear predictor for response. A terms specification of the form first + second indicates all the terms in first together with all the terms in second with any duplicates removed.

A specification of the form first:second indicates the set of terms obtained by taking the interactions of all terms in first with all terms in second. The specification first\*second indicates the cross of first and second. This is the same as first + second + first:second.

The terms in the formula will be re-ordered so that main effects come first, followed by the interactions, all second-order, all third-order and so on: to avoid this pass a terms object as the formula.

Non-NULL weights can be used to indicate that different observations have different dispersions (with the values in weights being inversely proportional to the dispersions); or equivalently, when the elements of weights are positive integers w\_i, that each response y\_i is the mean of w\_i unit-weight observations.

The default estimator for Degrees of Freedom is the Kramer and Sugiyama's one which only works for classical plsR models. For these models, Information criteria are computed accordingly to these estimations. Naive Degrees of Freedom and Information Criteria are also provided for comparison purposes. For more details, see N. Kraemer and M. Sugiyama. (2011). The Degrees of Freedom of Partial Least Squares Regression. *Journal of the American Statistical Association*, 106(494), 697-705, 2011.

#### Value

Depends on the model that was used to fit the model. You can generally at least find these items.

nr Number of observations nc Number of predictors

nt Number of requested components
ww raw weights (before L2-normalization)

wwnorm L2 normed weights (to be used with deflated matrices of predictor variables)
wwetoile modified weights (to be used with original matrix of predictor variables)

tt PLS components

pp loadings of the predictor variables

CoeffC coefficients of the PLS components
uscores scores of the response variable

YChapeau predicted response values for the dataX set

residYChapeau residuals of the deflated response on the standardized scale

RepY scaled response vector

na.miss.Y is there any NA value in the response vector YNA indicatrix vector of missing values in RepY

residY deflated scaled response vector ExpliX scaled matrix of predictors

na.miss.X is there any NA value in the predictor matrix XXNA indicator of non-NA values in the predictor matrix

residXX deflated predictor matrix

PredictY response values with NA replaced with 0
RSS residual sum of squares (original scale)
RSSresidY residual sum of squares (scaled scale)

R2 residY R2 coefficient value on the standardized scale
R2 R2 coefficient value on the original scale

press.ind individual PRESS value for each observation (scaled scale)
press.tot total PRESS value for all observations (scaled scale)

Q2cum cumulated Q2 (standardized scale)
family glm family used to fit PLSGLR model

ttPredictY PLS components for the dataset on which prediction was requested

typeVC type of leave one out cross-validation used

dataX predictor values dataY response values

weights weights of the observations

computed\_nt number of components that were computed

AIC AIC vs number of components
BIC BIC vs number of components

# Coeffsmodel\_vals

ChisqPearson

CoeffCFull matrix of the coefficients of the predictors

CoeffConstante value of the intercept (scaled scale)

Std. Coeffs Vector of standardized regression coefficients

Coeffs Vector of regression coefficients (used with the original data scale)

Yresidus residuals of the PLS model

residusY residuals of the deflated response on the standardized scale

InfCrit table of Information Criteria:

AIC AIC vs number of components BIC BIC vs number of components

MissClassed Number of miss classed results Chi2\_Pearson\_Y Q2 value (standardized scale) RSS residual sum of squares (original scale) R2 R2 coefficient value on the original scale

R2residY R2 coefficient value on the standardized scale

RSSresidY residual sum of squares (scaled scale)

Std.ValsPredictY

predicted response values for supplementary dataset (standardized scale)

ValsPredictY predicted response values for supplementary dataset (original scale)

Std. XChapeau estimated values for missing values in the predictor matrix (standardized scale)

FinalModel final GLR model on the PLS components

XXwotNA predictor matrix with missing values replaced with 0

call call

AIC.std AIC.std vs number of components (AIC computed for the standardized model

# Note

Use cv.plsRglm to cross-validate the plsRglm models and bootpls to bootstrap them.

### Author(s)

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http://www-irma.u-strasbg.fr/~fbertran/

#### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparaison de la regression PLS et de la regression logistique PLS: application aux donnees d'allelotypage. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

#### See Also

See also plsR.

```
data(Cornell)
XCornell<-Cornell[,1:7]</pre>
yCornell<-Cornell[,8]
modplsglm <- plsRglm(yCornell, XCornell, 10, modele="pls-glm-gaussian")</pre>
#To retrieve the final GLR model on the PLS components
finalmod <- plsRglm(yCornell,XCornell,10,modele="pls-glm-gaussian")$FinalModel</pre>
#It is a glm object.
plot(finalmod)
#Cross validation
cv.modplsglm<-cv.plsRglm(yCornell,XCornell,6,NK=100,modele="pls-glm-gaussian")
res.cv.modplsglm<-cvtable(summary(cv.modplsglm))</pre>
plot(res.cv.modplsglm)
#If no model specified, classic PLSR model
modpls <- plsRglm(yCornell, XCornell, 6)</pre>
modpls
modpls$tt
modpls$uscores
modpls$pp
modpls$Coeffs
#rm(list=c("XCornell","yCornell",modpls,cv.modplsglm,res.cv.modplsglm))
data(aze_compl)
Xaze_compl<-aze_compl[,2:34]</pre>
yaze_compl<-aze_compl$y</pre>
plsRglm(yaze_compl, Xaze_compl, nt=10, modele="pls", MClassed=TRUE) $InfCrit
modpls <- plsRglm(yaze_compl, Xaze_compl, nt=10, modele="pls-glm-logistic",</pre>
MClassed=TRUE,pvals.expli=TRUE)
modpls
colSums(modpls$pvalstep)
modpls$Coeffsmodel_vals
plot(plsRglm(yaze_compl, Xaze_compl, 4, modele="pls-glm-logistic")$FinalModel)
plsRglm(yaze_compl[-c(99,72)], Xaze_compl[-c(99,72),],4,
\verb|modele="pls-glm-logistic",pvals.expli=TRUE| \verb|spvalstep||
plot(plsRglm(yaze_compl[-c(99,72)], Xaze_compl[-c(99,72),],4,
modele="pls-glm-logistic",pvals.expli=TRUE)$FinalModel)
rm(list=c("Xaze_compl","yaze_compl","modpls"))
data(bordeaux)
Xbordeaux<-bordeaux[,1:4]</pre>
ybordeaux<-factor(bordeaux$Quality,ordered=TRUE)</pre>
\verb|modpls| <- plsRglm(ybordeaux,Xbordeaux,10,modele="pls-glm-polr",pvals.expli=TRUE)| \\
modpls
colSums(modpls$pvalstep)
XbordeauxNA<-Xbordeaux
```

```
XbordeauxNA[1,1] <- NA</pre>
modplsNA <- plsRglm(ybordeaux,XbordeauxNA,10,modele="pls-glm-polr",pvals.expli=TRUE)</pre>
modpls
colSums(modpls$pvalstep)
rm(list=c("Xbordeaux","XbordeauxNA","ybordeaux","modplsNA"))
data(pine)
Xpine<-pine[,1:10]</pre>
ypine<-pine[,11]</pre>
modpls1 <- plsRglm(ypine, Xpine, 1)</pre>
modpls1$Std.Coeffs
modpls1$Coeffs
modpls4 <- plsRglm(ypine, Xpine, 4)</pre>
modpls4$Std.Coeffs
modpls4$Coeffs
modpls4$PredictY[1,]
plsRglm(ypine,Xpine,4,dataPredictY=Xpine[1,])$PredictY[1,]
XpineNAX21 <- Xpine</pre>
XpineNAX21[1,2] <- NA
modpls4NA <- plsRglm(ypine,XpineNAX21,4)</pre>
modpls4NA$Std.Coeffs
modpls4NA$YChapeau[1,]
modpls4$YChapeau[1,]
modpls4NA$CoeffC
plsRglm(ypine,XpineNAX21,4,EstimXNA=TRUE)$XChapeau
plsRglm(ypine,XpineNAX21,4,EstimXNA=TRUE)$XChapeauNA
# compare pls-glm-gaussian with classic plsR
modplsglm4 <- plsRglm(ypine, Xpine, 4, modele="pls-glm-gaussian")</pre>
cbind(modpls4$Std.Coeffs,modplsglm4$Std.Coeffs)
# without missing data
cbind(ypine,modpls4$ValsPredictY,modplsglm4$ValsPredictY)
# with missing data
modplsglm4NA <- plsRglm(ypine,XpineNAX21,4,modele="pls-glm-gaussian")</pre>
cbind((ypine),modpls4NA$ValsPredictY,modplsglm4NA$ValsPredictY)
rm(list=c("Xpine","ypine","modpls4","modpls4NA","modplsglm4","modplsglm4NA"))
data(fowlkes)
Xfowlkes <- fowlkes[,2:13]</pre>
yfowlkes <- fowlkes[,1]</pre>
modpls <- plsRglm(yfowlkes,Xfowlkes,4,modele="pls-glm-logistic",pvals.expli=TRUE)</pre>
modpls
colSums(modpls$pvalstep)
rm(list=c("Xfowlkes", "yfowlkes", "modpls"))
if(require(chemometrics)){
data(hyptis)
yhyptis <- factor(hyptis$Group,ordered=TRUE)</pre>
Xhyptis <- as.data.frame(hyptis[,c(1:6)])</pre>
options(contrasts = c("contr.treatment", "contr.poly"))
modpls2 <- plsRglm(yhyptis, Xhyptis, 6, modele="pls-glm-polr")</pre>
modpls2$Coeffsmodel_vals
```

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```
modpls2$InfCrit
modpls2$Coeffs
modpls2$Std.Coeffs
table(yhyptis,predict(modpls2$FinalModel,type="class"))
rm(list=c("yhyptis","Xhyptis","modpls2"))
}
dimX <- 24
Astar <- 6
dataAstar6 <- t(replicate(250,simul_data_UniYX(dimX,Astar)))</pre>
ysimbin1 <- dicho(dataAstar6)[,1]</pre>
Xsimbin1 <- dicho(dataAstar6)[,2:(dimX+1)]</pre>
modplsglm <- plsRglm(ysimbin1, Xsimbin1, 10, modele="pls-glm-logistic")</pre>
modplsglm
cv.modplsglm <- cv.plsRglm(ysimbin1, Xsimbin1, nt=10,</pre>
modele="pls-glm-logistic",NK=100)
res.cv.modplsglm <- cvtable(summary(cv.modplsglm,MClassed=TRUE))</pre>
plot(res.cv.modplsglm) #defaults to type="CVMC"
rm(list=c("dimX", "Astar", "dataAstar6", "ysimbin1", "Xsimbin1", "modplsglm", "cv.modplsglm",
"res.cv.modplsglm"))
```

PLS\_glm\_wvc

*Light version of PLS\\_glm for cross validation purposes* 

#### **Description**

Light version of PLS\_glm for cross validation purposes either on complete or incomplete datasets.

# Usage

```
PLS_glm_wvc(dataY, dataX, nt = 2, dataPredictY = dataX, modele = "pls", family = NULL, scaleX = TRUE, scaleY = NULL, keepcoeffs = FALSE, keepstd.coeffs=FALSE, tol_Xi = 10^(-12), weights, method = "logistic", verbose = TRUE)
```

#### **Arguments**

dataY response (training) dataset

dataX predictor(s) (training) dataset

nt number of components to be extracted

dataPredictY predictor(s) (testing) dataset

modele name of the PLS glm model to be fitted ("pls", "pls-glm-Gamma", "pls-glm-gaussian", "pls-glm-inverse.gaussian", "pls-glm-logistic", "pls-glm-poisson", "pls-glm-polr"). Use "modele=pls-glm-family" to enable the family option.

family a description of the error distribution and link function to be used in the model.

This can be a character string naming a family function, a family function or the result of a call to a family function. (See family for details of family functions.)

To use the family option, please set modele="pls-glm-family". User defined

families can also be defined. See details.

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scaleX scale the predictor(s): must be set to TRUE for modele="pls" and should be for glms pls. scaleY scale the response: Yes/No. Ignored since non always possible for glm responses. keepcoeffs whether the coefficients of the linear fit on link scale of unstandardized eXplanatory variables should be returned or not. keepstd.coeffs whether the coefficients of the linear fit on link scale of standardized eXplanatory variables should be returned or not. tol\_Xi minimal value for Norm2(Xi) and  $det(pp' \times pp)$  if there is any missing value in the dataX. It defaults to  $10^{-12}$ an optional vector of 'prior weights' to be used in the fitting process. Should be weights NULL or a numeric vector. method logistic, probit, complementary log-log or cauchit (corresponding to a Cauchy latent variable). should info messages be displayed? verbose

#### **Details**

This function is called by PLS\_glm\_kfoldcv\_formula in order to perform cross-validation either on complete or incomplete datasets.

There are seven different predefined models with predefined link functions available:

"pls" ordinary pls models

"pls-glm-Gamma" glm gaussian with inverse link pls models

"pls-glm-gaussian" glm gaussian with identity link pls models

"pls-glm-inverse-gamma" glm binomial with square inverse link pls models

"pls-glm-logistic" glm binomial with logit link pls models

"pls-glm-poisson" glm poisson with log link pls models

"pls-glm-polr" glm polr with logit link pls models

Using the "family=" option and setting "modele=pls-glm-family" allows changing the family and link function the same way as for the glm function. As a consequence user-specified families can also be used.

The gaussian family accepts the links (as names) identity, log and inverse.

**The** binomial **family** accepts the links logit, probit, cauchit, (corresponding to logistic, normal and Cauchy CDFs respectively) log and cloglog (complementary log-log).

The Gamma family accepts the links inverse, identity and log.

**The** poisson **family** accepts the links log, identity, and sqrt.

The inverse gaussian family accepts the links 1/mu^2, inverse, identity and log.

**The** quasi **family** accepts the links logit, probit, cloglog, identity, inverse, log, 1/mu<sup>2</sup> and sqrt.

**The function** power can be used to create a power link function.

Non-NULL weights can be used to indicate that different observations have different dispersions (with the values in weights being inversely proportional to the dispersions); or equivalently, when the elements of weights are positive integers w\_i, that each response y\_i is the mean of w\_i unit-weight observations.

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#### Value

```
valsPredict nrow(dataPredictY) * nt matrix of the predicted values

coeffs If the coefficients of the eXplanatory variables were requested:
i.e. keepcoeffs=TRUE.
```

ncol(dataX) \* 1 matrix of the coefficients of the the eXplanatory variables

# Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

#### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

#### See Also

PLS\_glm for more detailed results, PLS\_glm\_kfoldcv for cross-validating models and PLS\_lm\_wvc for the same function dedicated to plsR models

```
data(Cornell)
XCornell<-Cornell[,1:7]</pre>
yCornell<-Cornell[,8]
PLS_glm_wvc(dataY=yCornell,dataX=XCornell,nt=3,modele="pls-glm-gaussian",
dataPredictY=XCornell[1,])
PLS_glm_wvc(dataY=yCornell,dataX=XCornell,nt=3,modele="pls-glm-family",
family=gaussian(),dataPredictY=XCornell[1,])
PLS\_glm\_wvc(dataY=yCornell[-1], dataX=XCornell[-1,], nt=3, modele="pls-glm-gaussian", nt=3, model
dataPredictY=XCornell[1,])
PLS_glm_wvc(dataY=yCornell[-1],dataX=XCornell[-1,],nt=3,modele="pls-glm-family",
family=gaussian(),dataPredictY=XCornell[1,])
rm("XCornell","yCornell")
## With an incomplete dataset (X[1,2] is NA)
data(pine)
ypine <- pine[,11]</pre>
data(XpineNAX21)
PLS_glm_wvc(dataY=ypine,dataX=XpineNAX21,nt=10,modele="pls-glm-gaussian")
rm("XpineNAX21","ypine")
data(pine)
Xpine<-pine[,1:10]</pre>
ypine<-pine[,11]</pre>
PLS_glm_wvc(ypine,Xpine,10,modele="pls")
PLS_glm_wvc(ypine,Xpine,10,modele="pls-glm-Gamma")
PLS_glm_wvc(ypine, Xpine, 10, modele="pls-glm-family", family=Gamma())
PLS_glm_wvc(ypine, Xpine, 10, modele="pls-glm-gaussian")
PLS_glm_wvc(ypine,Xpine,10,modele="pls-glm-family",family=gaussian(log))
```

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```
PLS_glm_wvc(round(ypine), Xpine, 10, modele="pls-glm-poisson")
PLS_glm_wvc(round(ypine), Xpine,10, modele="pls-glm-family", family=poisson(log))
rm(list=c("pine","ypine","Xpine"))
data(Cornell)
XCornell<-Cornell[,1:7]</pre>
yCornell<-Cornell[,8]
PLS_glm_wvc(yCornell, XCornell, 10, modele="pls-glm-inverse.gaussian")
PLS_glm_wvc(yCornell,XCornell,10,modele="pls-glm-family",
family=inverse.gaussian())
rm(list=c("XCornell","yCornell"))
data(Cornell)
XCornell<-Cornell[,1:7]</pre>
yCornell<-Cornell[,8]
PLS_glm_wvc(dataY=yCornell,dataX=XCornell,nt=3,modele="pls-glm-gaussian",
dataPredictY=XCornell[1,])
PLS_glm_wvc(dataY=yCornell[-1],dataX=XCornell[-1,],nt=3,modele="pls-glm-gaussian",
dataPredictY=XCornell[1,])
rm("XCornell","yCornell")
data(aze_compl)
Xaze_compl<-aze_compl[,2:34]</pre>
yaze_compl<-aze_compl$y</pre>
PLS_glm(yaze_compl,Xaze_compl,10,modele="pls-glm-logistic",typeVC="none")$InfCrit
PLS_glm_wvc(yaze_compl, Xaze_compl, 10, modele="pls-glm-logistic", keepcoeffs=TRUE)
rm("Xaze_compl","yaze_compl")
```

PLS\_1m\_wvc

*Light version of PLS*\\_lm for cross validation purposes

# Description

Light version of PLS\_1m for cross validation purposes either on complete or incomplete datasets.

# Usage

```
PLS_lm_wvc(dataY, dataX, nt = 2, dataPredictY = dataX, modele = "pls", scaleX = TRUE, scaleY = NULL, keepcoeffs = FALSE, keepstd.coeffs=FALSE, tol_Xi = 10^(-12), weights, verbose=TRUE)
```

# **Arguments**

dataY response (training) dataset
dataX predictor(s) (training) dataset

nt number of components to be extracted

dataPredictY predictor(s) (testing) dataset

modele name of the PLS model to be fitted, only ("pls" available for this fonction.

PLS\_lm\_wvc

scaleX	scale the predictor(s) : must be set to TRUE for $modele="pls"$ and should be for glms pls.
scaleY	scale the response : Yes/No. Ignored since non always possible for glm responses.
keepcoeffs	whether the coefficients of unstandardized eXplanatory variables should be returned or not.
keepstd.coeffs	whether the coefficients of standardized eXplanatory variables should be returned or not.
tol_Xi	minimal value for Norm2(Xi) and $\det(pp'\times pp)$ if there is any missing value in the dataX. It defaults to $10^{-12}$
weights	an optional vector of 'prior weights' to be used in the fitting process. Should be NULL or a numeric vector.

# **Details**

verbose

This function is called by PLS\_lm\_kfoldcv in order to perform cross-validation either on complete or incomplete datasets.

Non-NULL weights can be used to indicate that different observations have different dispersions (with the values in weights being inversely proportional to the dispersions); or equivalently, when the elements of weights are positive integers w\_i, that each response y\_i is the mean of w\_i unitweight observations.

#### Value

valsPredict nrow(dataPredictY) \* nt matrix of the predicted values coeffs If the coefficients of the eXplanatory variables were requested:

should info messages be displayed?

i.e. keepcoeffs=TRUE.

ncol(dataX) \* 1 matrix of the coefficients of the the eXplanatory variables

#### Note

Use PLS\_lm\_kfoldcv for a wrapper in view of cross-validation.

#### Author(s)

```
Frederic Bertrand
<frederic.bertrand@math.unistra.fr>
http://www-irma.u-strasbg.fr/~fbertran/
```

# References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. Journal de la Societe Française de Statistique, 151(2), pages 1-18. http://publications-sfds.math. cnrs.fr/index.php/J-SFdS/article/view/47

### See Also

PLS\_lm for more detailed results, PLS\_lm\_kfoldcv for cross-validating models and PLS\_glm\_wvc for the same function dedicated to plsRglm models

predict.plsRglmmodel

#### **Examples**

```
data(Cornell)
XCornell<-Cornell[,1:7]</pre>
yCornell<-Cornell[,8]
PLS_lm_wvc(dataY=yCornell,dataX=XCornell,nt=3,dataPredictY=XCornell[1,])
PLS_lm_wvc(dataY=yCornell[-c(1,2)], dataX=XCornell[-c(1,2),], nt=3, dataPredictY=XCornell[c(1,2),])
PLS_lm_wvc(dataY=yCornell[-c(1,2)], dataX=XCornell[-c(1,2),], nt=3, dataPredictY=XCornell[c(1,2),], nt=3, 
keepcoeffs=TRUE)
rm("XCornell","yCornell")
## With an incomplete dataset (X[1,2] is NA)
data(pine)
ypine <- pine[,11]</pre>
data(XpineNAX21)
PLS_lm_wvc(dataY=ypine[-1],dataX=XpineNAX21[-1,],nt=3)
PLS_lm_wvc(dataY=ypine[-1],dataX=XpineNAX21[-1,],nt=3,dataPredictY=XpineNAX21[1,])
PLS_lm_wvc(dataY=ypine[-2],dataX=XpineNAX21[-2,],nt=3,dataPredictY=XpineNAX21[2,])
PLS_lm_wvc(dataY=ypine,dataX=XpineNAX21,nt=3)
rm("XpineNAX21","ypine")
```

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#### **Description**

This function provides a predict method for the class "plsRglmmodel"

# Usage

```
## S3 method for class 'plsRglmmodel'
predict(object,newdata,comps=object$computed_nt,
type=c("link", "response", "terms", "scores", "class", "probs"),
se.fit=FALSE,weights, dispersion = NULL,methodNA="adaptative",verbose=TRUE,...)
```

#### **Arguments**

object	An object of the class "plsRmodel".
newdata	An optional data frame in which to look for variables with which to predict. If omitted, the fitted values are used.
comps	A value with a single value of component to use for prediction.
type	Type of predicted value. Available choices are the glms ones ("link", "response", "terms"), the polr ones ("class", "probs") or the scores ("scores").
se.fit	If TRUE, pointwise standard errors are produced for the predictions using the Cox model.
weights	Vector of case weights. If weights is a vector of integers, then the estimated coefficients are equivalent to estimating the model from data with the individual cases replicated as many times as indicated by weights.
dispersion	the dispersion of the GLM fit to be assumed in computing the standard errors. If omitted, that returned by summary applied to the object is used.

methodNA Selects the way of predicting the response or the scores of the new data. For

complete rows, without any missing value, there are two different ways of computing the prediction. As a consequence, for mixed datasets, with complete and incomplete rows, there are two ways of computing prediction: either predicts any row as if there were missing values in it (missingdata) or selects the pre-

diction method accordingly to the completeness of the row (adaptative).

verbose should info messages be displayed?

Arguments to be passed on to stats::glm and plsRglm::plsRglm.

#### Value

When type is "response", a matrix of predicted response values is returned. When type is "scores", a score matrix is returned.

#### Author(s)

```
Frederic Bertrand
<frederic.bertrand@math.unistra.fr>
http://www-irma.u-strasbg.fr/~fbertran/
```

#### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. Journal de la Societe Française de Statistique, 151(2), pages 1-18. http://publications-sfds.math. cnrs.fr/index.php/J-SFdS/article/view/47

### See Also

See Also predict.glm

```
data(pine)
Xpine<-pine[,1:10]</pre>
ypine<-pine[,11]</pre>
data(pine_sup)
Xpine_sup<-pine_sup[,1:10]</pre>
Xpine_supNA<-Xpine_sup</pre>
Xpine_supNA[1,1]<-NA</pre>
modpls=plsRglm(dataY=ypine,dataX=Xpine,nt=6,modele="pls-glm-family",family="gaussian")
modplsform=plsRglm(x11~.,data=pine,nt=6,modele="pls-glm-family",family="gaussian")
modpls2=plsRglm(dataY=ypine,dataX=Xpine,nt=6,modele="pls-glm-family",
dataPredictY=Xpine_sup,family="gaussian")
modpls2NA=plsRglm(dataY=ypine,dataX=Xpine,nt=6,modele="pls-glm-family",
dataPredictY=Xpine_supNA,family="gaussian")
#Identical to predict(modpls,type="link") or modpls$Std.ValsPredictY
cbind(modpls$Std.ValsPredictY,modplsform$Std.ValsPredictY,
predict(modpls),predict(modplsform))
#Identical to predict(modpls,type="response") or modpls$ValsPredictY
cbind(modpls$ValsPredictY,modplsform$ValsPredictY,
predict(modpls,type="response"),predict(modplsform,type="response"))
```

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```
#Identical to modpls$ttPredictY
predict(modpls,type="scores")
predict(modplsform, type="scores")
#Identical to modpls2$ValsPredictY
cbind(predict(modpls,newdata=Xpine_sup,type="response"),
predict(modplsform, newdata=Xpine_sup, type="response"))
#Select the number of components to use to derive the prediction
predict(modpls,newdata=Xpine_sup,type="response",comps=1)
predict(modpls,newdata=Xpine_sup,type="response",comps=3)
predict(modpls,newdata=Xpine_sup,type="response",comps=6)
try(predict(modpls,newdata=Xpine_sup,type="response",comps=8))
#Identical to modpls2$ttValsPredictY
predict(modpls,newdata=Xpine_sup,type="scores")
#Select the number of components in the scores matrix
predict(modpls,newdata=Xpine_sup,type="scores",comps=1)
predict(modpls,newdata=Xpine_sup,type="scores",comps=3)
predict(modpls,newdata=Xpine_sup,type="scores",comps=6)
try(predict(modpls, newdata=Xpine_sup, type="scores", comps=8))
#Identical to modpls2NA$ValsPredictY
predict(modpls,newdata=Xpine_supNA,type="response",methodNA="missingdata")
cbind(predict(modpls,newdata=Xpine_supNA,type="response"),
predict(modplsform, newdata=Xpine_supNA, type="response"))
predict(modpls,newdata=Xpine_supNA,type="response",comps=1)
predict(modpls,newdata=Xpine_supNA,type="response",comps=3)
predict(modpls, newdata=Xpine_supNA, type="response", comps=6)
try(predict(modpls,newdata=Xpine_supNA,type="response",comps=8))
#Identical to modpls2NA$ttPredictY
predict(modpls,newdata=Xpine_supNA,type="scores",methodNA="missingdata")
predict(modplsform,newdata=Xpine_supNA,type="scores",methodNA="missingdata")
predict(modpls,newdata=Xpine_supNA,type="scores")
predict(modplsform, newdata=Xpine_supNA, type="scores")
predict(modpls, newdata=Xpine_supNA, type="scores", comps=1)
predict(modpls,newdata=Xpine_supNA,type="scores",comps=3)
predict(modpls,newdata=Xpine_supNA,type="scores",comps=6)
try(predict(modpls,newdata=Xpine_supNA,type="scores",comps=8))
```

predict.plsRmodel

Print method for plsRcox models

#### **Description**

This function provides a predict method for the class "plsRcoxmodel"

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#### **Usage**

```
## S3 method for class 'plsRmodel'
predict(object, newdata, comps=object$computed_nt,
type=c("response","scores"),weights,methodNA="adaptative",verbose=TRUE,...)
```

#### **Arguments**

An object of the class "plsRmodel". object

An optional data frame in which to look for variables with which to predict. If newdata

omitted, the fitted values are used.

comps A value with a single value of component to use for prediction.

type Type of predicted value. Available choices are the response values ("response")

or the scores ("scores").

weights Vector of case weights. If weights is a vector of integers, then the estimated

coefficients are equivalent to estimating the model from data with the individual

cases replicated as many times as indicated by weights.

methodNA Selects the way of predicting the response or the scores of the new data. For

> complete rows, without any missing value, there are two different ways of computing the prediction. As a consequence, for mixed datasets, with complete and incomplete rows, there are two ways of computing prediction: either predicts any row as if there were missing values in it (missingdata) or selects the prediction method accordingly to the completeness of the row (adaptative).

should info messages be displayed? verbose

Arguments to be passed on to plsRglm::plsR. . . .

# Value

When type is "response", a matrix of predicted response values is returned. When type is "scores", a score matrix is returned.

### Author(s)

```
Frederic Bertrand
<frederic.bertrand@math.unistra.fr>
http://www-irma.u-strasbg.fr/~fbertran/
```

# References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. Journal de la Societe Française de Statistique, 151(2), pages 1-18. http://publications-sfds.math. cnrs.fr/index.php/J-SFdS/article/view/47

```
data(pine)
Xpine<-pine[,1:10]</pre>
ypine<-pine[,11]</pre>
data(pine_sup)
Xpine_sup<-pine_sup[,1:10]</pre>
Xpine_supNA<-Xpine_sup</pre>
```

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```
Xpine_supNA[1,1]<-NA
modpls=plsR(dataY=ypine,dataX=Xpine,nt=6,modele="pls")
modplsform=plsR(x11~.,data=pine,nt=6,modele="pls")
modpls2=plsR(dataY=ypine,dataX=Xpine,nt=6,modele="pls",dataPredictY=Xpine_sup)
modpls2NA=plsR(dataY=ypine,dataX=Xpine,nt=6,modele="pls",dataPredictY=Xpine_supNA)
#Identical to predict(modpls,type="response") or modpls$ValsPredictY
cbind(predict(modpls),predict(modplsform))
#Identical to modpls$ttPredictY
predict(modpls,type="scores")
predict(modplsform, type="scores")
#Identical to modpls2$ValsPredictY
cbind(predict(modpls,newdata=Xpine_sup,type="response"),
predict(modplsform,newdata=Xpine_sup,type="response"))
#Select the number of components to use to derive the prediction
predict(modpls,newdata=Xpine_sup,type="response",comps=1)
predict(modpls,newdata=Xpine_sup,type="response",comps=3)
predict(modpls,newdata=Xpine_sup,type="response",comps=6)
try(predict(modpls, newdata=Xpine_sup, type="response", comps=8))
#Identical to modpls2$ttValsPredictY
predict(modpls,newdata=Xpine_sup,type="scores")
#Select the number of components in the scores matrix
predict(modpls,newdata=Xpine_sup,type="scores",comps=1)
predict(modpls,newdata=Xpine_sup,type="scores",comps=3)
predict(modpls,newdata=Xpine_sup,type="scores",comps=6)
try(predict(modpls, newdata=Xpine_sup, type="scores", comps=8))
#Identical to modpls2NA$ValsPredictY
predict(modpls,newdata=Xpine_supNA,type="response",methodNA="missingdata")
cbind(predict(modpls,newdata=Xpine_supNA,type="response"),
predict(modplsform, newdata=Xpine_supNA, type="response"))
predict(modpls, newdata=Xpine_supNA, type="response", comps=1)
predict(modpls,newdata=Xpine_supNA,type="response",comps=3)
predict(modpls,newdata=Xpine_supNA,type="response",comps=6)
try(predict(modpls,newdata=Xpine_supNA,type="response",comps=8))
#Identical to modpls2NA$ttPredictY
predict(modpls,newdata=Xpine_supNA,type="scores",methodNA="missingdata")
predict(modplsform,newdata=Xpine_supNA,type="scores",methodNA="missingdata")
predict(modpls,newdata=Xpine_supNA,type="scores")
predict(modplsform,newdata=Xpine_supNA,type="scores")
predict(modpls,newdata=Xpine_supNA,type="scores",comps=1)
predict(modpls,newdata=Xpine_supNA,type="scores",comps=3)
predict(modpls,newdata=Xpine_supNA,type="scores",comps=6)
try(predict(modpls, newdata=Xpine_supNA, type="scores", comps=8))
```

```
print.coef.plsRglmmodel
```

Print method for plsRglm models

# Description

This function provides a print method for the class "coef.plsRglmmodel"

# Usage

```
## S3 method for class 'coef.plsRglmmodel'
print(x, ...)
```

# **Arguments**

```
x an object of the class "coef.plsRglmmodel"
... not used
```

#### Value

NULL

#### Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

# References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

# See Also

print

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
modplsglm <- plsRglm(yCornell,XCornell,3,modele="pls-glm-family",family=gaussian())
class(modplsglm)
print(coef(modplsglm))
rm(list=c("XCornell","yCornell","modplsglm"))</pre>
```

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```
print.coef.plsRmodel Print method for plsR models
```

# Description

This function provides a print method for the class "coef.plsRmodel"

# Usage

```
## S3 method for class 'coef.plsRmodel'
print(x, ...)
```

# **Arguments**

```
x an object of the class "coef.plsRmodel"
... not used
```

#### Value

NULL

#### Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

### See Also

```
print
```

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
modpls <- plsRglm(yCornell, XCornell, 3, modele="pls")
class(modpls)
print(coef(modpls))
rm(list=c("XCornell", "yCornell", "modpls"))</pre>
```

```
print.cv.plsRglmmodel Print method for plsRglm models
```

# Description

This function provides a print method for the class "cv.plsRglmmodel"

# Usage

```
## S3 method for class 'cv.plsRglmmodel'
print(x, ...)
```

# **Arguments**

```
x an object of the class "cv.plsRglmmodel"
... not used
```

#### Value

NULL

#### Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

### References

Nicolas Meyer, Myriam Maumy-Bertrand et  $Fr\tilde{A}@d\tilde{A}$ @ric Bertrand (2010). Comparaison de la  $r\tilde{A}$ @gression PLS et de la r?gression logistique PLS : application aux donn?es d'all $\tilde{A}$ @lotypage. Journal de la  $Soci\tilde{A}@t\tilde{A}@Fran\tilde{A}$ §aise de Statistique, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

### See Also

```
print
```

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
bbb <- cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=10,NK=1,modele="pls-glm-family",family=gaussian())
print(bbb)
rm(list=c("XCornell","yCornell","bbb"))</pre>
```

print.cv.plsRmodel 95

print.cv.plsRmodel

Print method for plsR models

# **Description**

This function provides a print method for the class "cv.plsRmodel"

#### Usage

```
## S3 method for class 'cv.plsRmodel'
print(x, ...)
```

# **Arguments**

```
x an object of the class "cv.plsRmodel"
...
```

#### Value

NULL

# Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

# References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

### See Also

```
print
```

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
bbb <- cv.plsR(dataY=yCornell,dataX=XCornell,nt=10,K=6)
print(bbb)
rm(list=c("XCornell","yCornell","bbb"))</pre>
```

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print.plsRglmmodel

Print method for plsRglm models

# Description

This function provides a print method for the class "plsRglmmodel"

# Usage

```
## S3 method for class 'plsRglmmodel'
print(x, ...)
```

# **Arguments**

```
x an object of the class "plsRglmmodel"
... not used
```

#### Value

NULL

#### Author(s)

```
Fr?d?ric Bertrand
<frederic.bertrand@math.unistra.fr>
http://www-irma.u-strasbg.fr/~fbertran/
```

### References

Nicolas Meyer, Myriam Maumy-Bertrand et Fr?d?ric Bertrand (2010). Comparaison de la r?gression PLS et de la r?gression logistique PLS: application aux donn?es d'all?lotypage. *Journal de la Soci?t? Fran?aise de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

### See Also

```
print
```

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
modplsglm <- plsRglm(yCornell,XCornell,3,modele="pls-glm-gaussian")
class(modplsglm)
print(modplsglm)
rm(list=c("XCornell","yCornell","modplsglm"))</pre>
```

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print.plsRmodel

Print method for plsR models

# Description

This function provides a print method for the class "plsRmodel"

# Usage

```
## S3 method for class 'plsRmodel'
print(x, ...)
```

# **Arguments**

```
x an object of the class "plsRmodel"
... not used
```

#### Value

NULL

# Author(s)

```
Fr?d?ric Bertrand
<frederic.bertrand@math.unistra.fr>
http://www-irma.u-strasbg.fr/~fbertran/
```

### References

Nicolas Meyer, Myriam Maumy-Bertrand et Fr?d?ric Bertrand (2010). Comparaison de la r?gression PLS et de la r?gression logistique PLS: application aux donn?es d'all?lotypage. *Journal de la Soci?t? Fran?aise de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

### See Also

```
print
```

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
modpls <- plsRglm(yCornell, XCornell, 3, modele="pls")
class(modpls)
print(modpls)
rm(list=c("XCornell", "yCornell", "modpls"))</pre>
```

```
print.summary.plsRglmmodel
```

Print method for summaries of plsRglm models

# **Description**

This function provides a print method for the class "summary.plsRglmmodel"

# Usage

```
## S3 method for class 'summary.plsRglmmodel'
print(x, ...)
```

# **Arguments**

```
x an object of the class "summary.plsRglmmodel"
... not used
```

#### Value

language call of the model

# Author(s)

```
Fr?d?ric Bertrand
<frederic.bertrand@math.unistra.fr>
http://www-irma.u-strasbg.fr/~fbertran/
```

# References

Nicolas Meyer, Myriam Maumy-Bertrand et Fr?d?ric Bertrand (2010). Comparaison de la r?gression PLS et de la r?gression logistique PLS: application aux donn?es d'all?lotypage. *Journal de la Soci?t? Fran?aise de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

# See Also

```
print and summary
```

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
modplsglm <- plsRglm(yCornell,XCornell,3,modele="pls-glm-gaussian")
class(modplsglm)
print(summary(modplsglm))
rm(list=c("XCornell","yCornell","modplsglm"))</pre>
```

```
print.summary.plsRmodel
```

Print method for summaries of plsR models

# **Description**

This function provides a print method for the class "summary.plsRmodel"

# Usage

```
## S3 method for class 'summary.plsRmodel'
print(x, ...)
```

# Arguments

```
x an object of the class "summary.plsRmodel"
... not used
```

#### Value

language call of the model

# Author(s)

```
Fr?d?ric Bertrand
<frederic.bertrand@math.unistra.fr>
http://www-irma.u-strasbg.fr/~fbertran/
```

# References

Nicolas Meyer, Myriam Maumy-Bertrand et Fr?d?ric Bertrand (2010). Comparaison de la r?gression PLS et de la r?gression logistique PLS: application aux donn?es d'all?lotypage. *Journal de la Soci?t? Fran?aise de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

# See Also

```
print and summary
```

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
modpls <- plsRglm(yCornell, XCornell, 3, modele="pls")
class(modpls)
print(summary(modpls))
rm(list=c("XCornell", "yCornell", "modpls"))</pre>
```

100 signpred

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$^{\circ}$	511	$\mathbf{p}$	Cu

Graphical assessment of the stability of selected variables

# **Description**

This fonctions plots, for each of the model, the

# Usage

```
signpred(matbin, pred.lablength = max(sapply(rownames(matbin), nchar)),
labsize = 1, plotsize = 12)
```

#### **Arguments**

matbin Matrix with 0 or 1 entries. Each row per predictor and a column for every model.

0 means the predictor is not significant in the model and 1 that, on the contrary,

it is significant.

pred.lablength Maximum length of the predictors labels. Defaults to full label length.

labsize Size of the predictors labels.
plotsize Global size of the graph.

#### **Details**

This function is based on the visweb function from the bipartite package.

### Value

A plot window.

# Author(s)

```
Bernd Gruber with minor modifications from Frederic Bertrand <frederic.bertrand@math.unistra.fr> http://www-irma.u-strasbg.fr/~fbertran/
```

### References

Vazquez, P.D., Chacoff, N.,P. and Cagnolo, L. (2009) Evaluating multiple determinants of the structure of plant-animal mutualistic networks. *Ecology*, 90:2039-2046.

# See Also

See Also visweb

```
signpred(matrix(rbinom(160,1,.2),ncol=8,dimnames=list(as.character(1:20),as.character(1:8))))\\
```

simul\_data\_complete 101

# **Description**

This function generates a single multivariate response value Y and a vector of explinatory variables  $(X_1, \ldots, X_{totdim})$  drawn from a model with a given number of latent components.

# Usage

```
simul_data_complete(totdim, ncomp)
```

# **Arguments**

totdim	Number of columns of the X vector (from ncomp to hardware limits)
ncomp	Number of latent components in the model (from 2 to 6)

#### **Details**

This function should be combined with the replicate function to give rise to a larger dataset. The algorithm used is a R port of the one described in the article of Li which is a multivariate generalization of the algorithm of Naes and Martens.

#### Value

simX	Vector of explanatory variables
НН	Dimension of the response $\boldsymbol{Y}$
eta	See Li et al.
r	See Li et al.
epsilon	See Li et al.
ksi	See Li et al.
f	See Li et al.
z	See Li et al.
Υ	See Li et al.

# Note

The value of r depends on the value of ncomp :

ncomp	1
2	
3	
4	4

### Author(s)

```
Frederic Bertrand <frederic.bertrand@math.unistra.fr>
```

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```
http://www-irma.u-strasbg.fr/~fbertran/
```

#### References

T. Naes, H. Martens, Comparison of prediction methods for multicollinear data, Commun. Stat., Simul. 14 (1985) 545-576.

Baibing Li, Julian Morris, Elaine B. Martin, Model selection for partial least squares regression, Chemometrics and Intelligent Laboratory Systems 64 (2002) 79-89.

```
http://dx.doi.org/10.1016/S0169-7439(02)00051-5
```

#### See Also

```
simul_data_YX for data simulation purpose
```

#### **Examples**

```
simul_data_complete(20,6)

dimX <- 6
Astar <- 2
simul_data_complete(dimX,Astar)

dimX <- 6
Astar <- 3
simul_data_complete(dimX,Astar)

dimX <- 6
Astar <- 4
simul_data_complete(dimX,Astar)

rm(list=c("dimX","Astar"))</pre>
```

simul\_data\_UniYX

Data generating function for univariate plsR models

# Description

This function generates a single univariate response value Y and a vector of explanatory variables  $(X_1, \ldots, X_{totdim})$  drawn from a model with a given number of latent components.

#### Usage

```
simul_data_UniYX(totdim, ncomp)
```

### **Arguments**

totdim Number of columns of the X vector (from ncomp to hardware limits)

ncomp Number of latent components in the model (from 2 to 6)

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#### **Details**

This function should be combined with the replicate function to give rise to a larger dataset. The algorithm used is a R port of the one described in the article of Li which is a multivariate generalization of the algorithm of Naes and Martens.

#### Value

```
vector (Y, X_1, \dots, X_{totdim})
```

# Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

#### References

T. Naes, H. Martens, Comparison of prediction methods for multicollinear data, Commun. Stat., Simul. 14 (1985) 545-576.

Baibing Li, Julian Morris, Elaine B. Martin, Model selection for partial least squares regression, Chemometrics and Intelligent Laboratory Systems 64 (2002) 79-89.

```
http://dx.doi.org/10.1016/S0169-7439(02)00051-5
```

#### See Also

simul\_data\_YX and simul\_data\_complete for generating multivariate data

```
simul_data_UniYX(20,6)
dimX < - 6
Astar <- 2
simul_data_UniYX(dimX,Astar)
(dataAstar2 <- t(replicate(50,simul_data_UniYX(dimX,Astar))))</pre>
cvtable(summary(cv.plsR(dataAstar2[,1],dataAstar2[,2:7],5,NK=100)))
dimX < -6
Astar <- 3
simul_data_UniYX(dimX,Astar)
(dataAstar3 <- t(replicate(50,simul_data_UniYX(dimX,Astar))))</pre>
cvtable(summary(cv.plsR(dataAstar3[,1],dataAstar3[,2:7],5,NK=100)))
dimX < -6
Astar <- 4
simul_data_UniYX(dimX,Astar)
(dataAstar4 <- t(replicate(50,simul_data_UniYX(dimX,Astar))))</pre>
cvtable(summary(cv.plsR(dataAstar4[,1],dataAstar4[,2:7],5,NK=100)))
rm(list=c("dimX","Astar"))
```

simul\_data\_UniYX\_binom

Data generating function for univariate binomial plsR models

# **Description**

This function generates a single univariate binomial response value Y and a vector of explanatory variables  $(X_1, \ldots, X_{totdim})$  drawn from a model with a given number of latent components.

# Usage

```
simul_data_UniYX_binom(totdim, ncomp, link="logit", offset = 0)
```

#### **Arguments**

totdim	Number of columns of the X vector (from ncomp to hardware limits)
ncomp	Number of latent components in the model (from 2 to 6)
link	Character specification of the link function in the mean model (mu). Currently, "logit", "probit", "cloglog", "cauchit", "log", "loglog" are supported. Alternatively, an object of class "link-glm" can be supplied.

offset Offset on the linear scale

#### **Details**

This function should be combined with the replicate function to give rise to a larger dataset. The algorithm used is a modification of a R port of the one described in the article of Li which is a multivariate generalization of the algorithm of Naes and Martens.

### Value

```
vector (Y, X_1, \dots, X_{totdim})
```

#### Author(s)

```
Fr?d?ric Bertrand
<frederic.bertrand@math.unistra.fr>
http://www-irma.u-strasbg.fr/~fbertran/
```

# References

T. Naes, H. Martens, Comparison of prediction methods for multicollinear data, Commun. Stat., Simul. 14 (1985) 545-576.

Baibing Li, Julian Morris, Elaine B. Martin, Model selection for partial least squares regression, Chemometrics and Intelligent Laboratory Systems 64 (2002) 79-89.

```
http://dx.doi.org/10.1016/S0169-7439(02)00051-5
```

# See Also

```
simul_data_UniYX
```

simul\_data\_YX 105

```
layout(matrix(1:6,nrow=2))
# logit link
hist(t(replicate(100, simul_data_UniYX_binom(4,4)))[,1])
# probit link
hist(t(replicate(100, simul_data_UniYX_binom(4,4,link="probit")))[,1])
# cloglog link
hist(t(replicate(100,simul_data_UniYX_binom(4,4,link="cloglog")))[,1])
# cauchit link
hist(t(replicate(100,simul_data_UniYX_binom(4,4,link="cauchit")))[,1])
# loglog link
hist(t(replicate(100, simul_data_UniYX_binom(4,4,link="loglog")))[,1])
# log link
hist(t(replicate(100, simul_data_UniYX_binom(4,4,link="log")))[,1])
layout(1)
layout(matrix(1:6,nrow=2))
# logit link
hist(t(replicate(100, simul_data_UniYX_binom(4,4,offset=5)))[,1])
# probit link
hist(t(replicate(100,simul_data_UniYX_binom(4,4,link="probit",offset=5)))[,1])
# cloglog link
hist(t(replicate(100,simul_data_UniYX_binom(4,4,link="cloglog",offset=5)))[,1])
# cauchit link
hist(t(replicate(100,simul_data_UniYX_binom(4,4,link="cauchit",offset=5)))[,1])
# loglog link
\label{linear_log_log_problem} hist(t(replicate(100,simul\_data\_UniYX\_binom(4,4,link="loglog",offset=5)))[,1])
# log link
hist(t(replicate(100, simul_data_UniYX_binom(4,4,link="log",offset=5)))[,1])
layout(1)
layout(matrix(1:6,nrow=2))
# logit link
\label{limit} hist(t(replicate(100,simul\_data\_UniYX\_binom(4,4,offset=-5)))[,1])
# probit link
hist(t(replicate(100,simul_data_UniYX_binom(4,4,link="probit",offset=-5)))[,1])
# cloglog link
hist(t(replicate(100,simul_data_UniYX_binom(4,4,link="cloglog",offset=-5)))[,1])
# cauchit link
hist(t(replicate(100,simul_data_UniYX_binom(4,4,link="cauchit",offset=-5)))[,1])
# loglog link
hist(t(replicate(100,simul_data_UniYX_binom(4,4,link="loglog",offset=-5)))[,1])
hist(t(replicate(100,simul_data_UniYX_binom(4,4,link="log",offset=-5)))[,1])
layout(1)
```

simul\_data\_YX

#### **Description**

This function generates a single multivariate response value Y and a vector of explinatory variables  $(X_1, \ldots, X_{totdim})$  drawn from a model with a given number of latent components.

# Usage

```
simul_data_YX(totdim, ncomp)
```

# **Arguments**

totdim Number of column of the X vector (from ncomp to hardware limits)

ncomp Number of latent components in the model (from 2 to 6)

#### **Details**

This function should be combined with the replicate function to give rise to a larger dataset. The algorithm used is a R port of the one described in the article of Li which is a multivariate generalization of the algorithm of Naes and Martens.

#### Value

vector 
$$(Y_1, \ldots, Y_r, X_1, \ldots, X_{totdim})$$

#### Note

The value of r depends on the value of ncomp:

ncomp	$\gamma$
2	3
3	3
4	4

# Author(s)

Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/

#### References

T. Naes, H. Martens, Comparison of prediction methods for multicollinear data, Commun. Stat., Simul. 14 (1985) 545-576.

Baibing Li, Julian Morris, Elaine B. Martin, Model selection for partial least squares regression, Chemometrics and Intelligent Laboratory Systems 64 (2002) 79-89.

http://dx.doi.org/10.1016/S0169-7439(02)00051-5

# See Also

simul\_data\_complete for highlighting the simulations parameters

### **Examples**

```
simul_data_YX(20,6)
if(require(plsdepot)){
dimX < - 6
Astar <- 2
(dataAstar2 <- t(replicate(50,simul_data_YX(dimX,Astar))))</pre>
library(plsdepot)
resAstar2 <- plsreg2(dataAstar2[,4:9],dataAstar2[,1:3],comps=5)</pre>
resAstar2$Q2
resAstar2$Q2[,4]>0.0975
dimX < - 6
Astar <- 3
(dataAstar3 <- t(replicate(50,simul_data_YX(dimX,Astar))))</pre>
library(plsdepot)
resAstar3 <- plsreg2(dataAstar3[,4:9],dataAstar3[,1:3],comps=5)</pre>
resAstar3$Q2
resAstar3$Q2[,4]>0.0975
dimX < - 6
Astar <- 4
(dataAstar4 <- t(replicate(50, simul_data_YX(dimX, Astar))))</pre>
library(plsdepot)
resAstar4 <- plsreg2(dataAstar4[,5:10],dataAstar4[,1:4],comps=5)</pre>
resAstar4$Q2
resAstar4$Q2[,5]>0.0975
rm(list=c("dimX","Astar"))
}
```

```
summary.cv.plsRglmmodel
```

Summary method for plsRglm models

# **Description**

This function provides a summary method for the class "cv.plsRglmmodel"

### Usage

```
## S3 method for class 'cv.plsRglmmodel'
summary(object, ...)
```

# **Arguments**

```
object an object of the class "cv.plsRglmmodel"
... further arguments to be passed to or from methods.
```

#### Value

An object of class "summary.cv.plsRmodel" if model is missing or model="pls". Otherwise an object of class "summary.cv.plsRglmmodel".

#### Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

# References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

#### See Also

```
summary
```

# **Examples**

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
bbb <- cv.plsRglm(dataY=yCornell,dataX=XCornell,nt=10,NK=1,
modele="pls-glm-family",family=gaussian())
summary(bbb)
rm(list=c("XCornell","yCornell","bbb"))</pre>
```

summary.cv.plsRmodel Summary method for plsR models

# Description

This function provides a summary method for the class "cv.plsRmodel"

#### Usage

```
## S3 method for class 'cv.plsRmodel'
summary(object, ...)
```

### **Arguments**

```
object an object of the class "cv.plsRmodel"
... further arguments to be passed to or from methods.
```

#### Value

An object of class "summary.cv.plsRglmmodel".

#### Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

#### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

#### See Also

summary

# **Examples**

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
bbb <- cv.plsR(dataY=yCornell,dataX=XCornell,nt=10,K=6)
summary(bbb)
rm(list=c("XCornell","yCornell","bbb"))</pre>
```

summary.plsRglmmodel Summary method for plsRglm models

### **Description**

This function provides a summary method for the class "plsRglmmodel"

### Usage

```
## S3 method for class 'plsRglmmodel'
summary(object, ...)
```

# **Arguments**

```
object an object of the class "plsRglmmodel"
... further arguments to be passed to or from methods.
```

### Value

call function call of plsRglmmodel

# Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

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#### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

#### See Also

summary

# **Examples**

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
modplsglm <- plsRglm(yCornell,XCornell,3,modele="pls-glm-gaussian")
class(modplsglm)
summary(modplsglm)
rm(list=c("XCornell","yCornell","modplsglm"))</pre>
```

summary.plsRmodel

Summary method for plsR models

#### **Description**

This function provides a summary method for the class "plsRmodel"

#### Usage

```
## S3 method for class 'plsRmodel'
summary(object, ...)
```

# **Arguments**

object an object of the class "plsRmodel"
... further arguments to be passed to or from methods.

### Value

call function call of plsRmodel

### Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

#### References

Nicolas Meyer, Myriam Maumy-Bertrand et Frederic Bertrand (2010). Comparing the linear and the logistic PLS regression with qualitative predictors: application to allelotyping data. *Journal de la Societe Française de Statistique*, 151(2), pages 1-18. http://publications-sfds.math.cnrs.fr/index.php/J-SFdS/article/view/47

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#### See Also

```
summary
```

#### **Examples**

```
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]
modpls <- plsR(yCornell,XCornell,3,modele="pls")
class(modpls)
summary(modpls)
rm(list=c("XCornell","yCornell","modpls"))</pre>
```

tilt.bootpls

Tilted bootstrap for PLS models

# Description

```
~~ A (1-5 lines) description of what the function does. ~~
```

~~Explain object here~~

# Usage

```
tilt.bootpls(object, typeboot="plsmodel", statistic=coefs.plsR,
R=c(499, 250, 250), alpha=c(0.025, 0.975), sim="ordinary",
stype="i", index=1, stabvalue=1e6,...)
```

# **Arguments**

object

```
typeboot
                 ~~Explain typeboot here~~
                 ~~Explain statistic here~~
statistic
R
                 ~~Explain R here~~
alpha
                 ~~Explain alpha here~~
                 ~~Explain sim here~~
sim
                 ~~Explain stype here~~
stype
index
                 ~~Explain index here~~
                 ~~Explain stabvalue here~~
stabvalue
                 ~~Explain . . . here~~
. . .
```

#### **Details**

~~ More details than the description above ~~

# Value

~Describe the value returned If it is a LIST, use

```
comp1 Description of 'comp1' comp2 Description of 'comp2'
```

...

tilt.bootplsglm

### Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

#### See Also

```
tilt.boot
```

#### **Examples**

```
## Not run:
data(Cornell)
XCornell<-Cornell[,1:7]
yCornell<-Cornell[,8]

set.seed(1385)
Cornell.tilt.boot <- tilt.bootpls(plsR(yCornell,XCornell,3), statistic=coefs.plsR,
R=c(499, 100, 100), alpha=c(0.025, 0.975), sim="ordinary", stype="i", index=1)
Cornell.tilt.boot
str(Cornell.tilt.boot)

boxplots.bootpls(Cornell.tilt.boot,indices=2:7)

rm(Cornell.tilt.boot)

## End(Not run)</pre>
```

tilt.bootplsglm

Tilted bootstrap for PLS models

# Description

```
~~ A (1-5 lines) description of what the function does. ~~
```

~~Explain object here~~

# Usage

```
tilt.bootplsglm(object, typeboot="fmodel_np", statistic=coefs.plsRglm, R=c(499, 250, 250), alpha=c(0.025, 0.975), sim="ordinary", stype="i", index=1, stabvalue=1e6,...)
```

# Arguments

object

```
typeboot ~~Explain typeboot here~~
statistic ~~Explain statistic here~~
R ~~Explain R here~~
alpha ~~Explain alpha here~~
sim ~~Explain sim here~~
stype ~~Explain stype here~~
```

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```
index ~~Explain index here~~
stabvalue ~~Explain stabvalue here~~
... ~~Explain ... here~~
```

#### Details

~~ More details than the description above ~~

#### Value

```
~Describe the value returned If it is a LIST, use
```

```
comp1 Description of 'comp1' comp2 Description of 'comp2'
```

•••

### Author(s)

```
Frederic Bertrand

<frederic.bertrand@math.unistra.fr>

http://www-irma.u-strasbg.fr/~fbertran/
```

#### See Also

tilt.boot

```
data(aze_compl)
Xaze_compl<-aze_compl[,2:34]</pre>
yaze_compl<-aze_compl$y</pre>
dataset <- cbind(y=yaze_compl, Xaze_compl)</pre>
# Lazraq-Cleroux PLS bootstrap Classic
aze_compl.tilt.boot <- tilt.bootplsglm(plsRglm(yaze_compl,Xaze_compl,3,</pre>
modele="pls-glm-logistic", family=NULL), statistic=coefs.plsRglm, R=c(499, 100, 100),
alpha=c(0.025, 0.975), sim="ordinary", stype="i", index=1)
aze_compl.tilt.boot <- tilt.bootplsglm(plsRglm(yaze_compl,Xaze_compl,3,</pre>
modele="pls-glm-logistic"), statistic=coefs.plsRglm, R=c(499, 100, 100),
alpha=c(\texttt{0.025}, \texttt{ 0.975}), \texttt{ sim="ordinary"}, \texttt{ stype="i"}, \texttt{ index=1})
aze_compl.tilt.boot <- tilt.bootplsglm(plsRglm(yaze_compl, Xaze_compl, 3,</pre>
modele="pls-glm-family", family=binomial), statistic=coefs.plsRglm, R=c(499, 100, 100),
alpha=c(0.025, 0.975), sim="ordinary", stype="i", index=1)
boxplots.bootpls(aze_compl.tilt.boot,1:2)
# PLS bootstrap balanced
aze_compl.tilt.boot <- tilt.bootplsglm(plsRglm(yaze_compl,Xaze_compl,3,</pre>
modele="pls-glm-logistic"), statistic=coefs.plsRglm, R=c(499, 100, 100),
alpha=c(0.025, 0.975), sim="balanced", stype="i", index=1)
```

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XbordeauxNA

Incomplete dataset for the quality of wine dataset

# Description

Quality of Bordeaux wines (Quality) and four potentially predictive variables (Temperature, Sunshine, Heat and Rain).

The value of Temperature for the first observation was remove from the matrix of predictors on purpose.

# Usage

data(XbordeauxNA)

#### **Format**

A data frame with 34 observations on the following 4 variables.

Temperature a numeric vector

Sunshine a numeric vector

Heat a numeric vector

Rain a numeric vector

# Source

P. Bastien, V. Esposito-Vinzi, and M. Tenenhaus. (2005). PLS generalised linear regression. *Computational Statistics & Data Analysis*, 48(1):17-46.

#### References

M. Tenenhaus. (2005). La regression logistique PLS. In J.-J. Droesbeke, M. Lejeune, and G. Saporta, editors, Modeles statistiques pour donnees qualitatives. Editions Technip, Paris.

# **Examples**

data(XbordeauxNA)
str(XbordeauxNA)

XpineNAX21

XpineNAX21

*Incomplete dataset from the pine caterpillars example* 

### **Description**

The caterpillar dataset was extracted from a 1973 study on pine processionary caterpillars. It assesses the influence of some forest settlement characteristics on the development of caterpillar colonies. There are k=10 potentially explanatory variables defined on n=33 areas.

The value of x2 for the first observation was remove from the matrix of predictors on purpose.

# Usage

```
data(XpineNAX21)
```

#### **Format**

A data frame with 33 observations on the following 10 variables.

- x1 altitude (in meters)
- x2 slope (en degrees)
- x3 number of pines in the area
- x4 height (in meters) of the tree sampled at the center of the area
- x5 diameter (in meters) of the tree sampled at the center of the area
- x6 index of the settlement density
- x7 orientation of the area (from 1 if southbound to 2 otherwise)
- x8 height (in meters) of the dominant tree
- x9 number of vegetation strata
- x10 mix settlement index (from 1 if not mixed to 2 if mixed)

#### **Details**

These caterpillars got their names from their habit of moving over the ground in incredibly long head-to-tail processions when leaving their nest to create a new colony.

The XpineNAX21 is a dataset with a missing value for testing purpose.

#### Source

Tomassone R., Audrain S., Lesquoy-de Turckeim E., Millier C. (1992). "La regression, nouveaux regards sur une ancienne methode statistique", INRA, *Actualit?s Scientifiques et Agronomiques*, Masson, Paris.

```
data(XpineNAX21)
str(XpineNAX21)
```

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