

Package ‘gpls’

September 24, 2012

Title Classification using generalized partial least squares

Version 1.28.0

Author Beiyong Ding

Description Classification using generalized partial least squares
for two-group and multi-group (more than 2 group) classification.

Maintainer Bioconductor Package Maintainer <maintainer@bioconductor.org>

Imports stats

Suggests MASS

License Artistic-2.0

biocViews Bioinformatics, Classification, Microarray

R topics documented:

gpls1a	2
gpls1a.cv.error	3
gpls1a.logit.all	4
gpls1a.mlogit	5
gpls1a.mlogit.cv.error	6
gpls1a.train.test.error	7
gpls	8
predict.gpls	10

Index	12
--------------	-----------

glpls1a

*Fit IRWPLS and IRWPLSF model***Description**

Fit Iteratively ReWeighted Least Squares (IRWPLS) with an option of Firth's bias reduction procedure (IRWPLSF) for two-group classification

Usage

```
glpls1a(X, y, K.prov = NULL, eps = 0.001, lmax = 100, b.ini = NULL,
        denom.eps = 1e-20, family = "binomial", link = NULL, br = TRUE)
```

Arguments

X	n by p design matrix (with no intercept term)
y	response vector 0 or 1
K.prov	number of PLS components, default is the rank of X
eps	tolerance for convergence
lmax	maximum number of iteration allowed
b.ini	initial value of regression coefficients
denom.eps	small quantity to guarantee nonzero denominator in deciding convergence
family	glm family, binomial is the only relevant one here
link	link function, logit is the only one practically implemented now
br	TRUE if Firth's bias reduction procedure is used

Value

coefficients	regression coefficients
convergence	whether convergence is achieved
niter	total number of iterations
bias.reduction	whether Firth's procedure is used
loading.matrix	the matrix of loadings

Author(s)

Beiying Ding, Robert Gentleman

References

- Ding, B.Y. and Gentleman, R. (2003) *Classification using generalized partial least squares*.
- Marx, B.D (1996) Iteratively reweighted partial least squares estimation for generalized linear regression. *Technometrics* 38(4): 374-381.

See Also

[glpls1a.mlogit](#), [glpls1a.logit.all](#), [glpls1a.train.test.error](#), [glpls1a.cv.error](#), [glpls1a.mlogit.cv.error](#)

Examples

```
x <- matrix(rnorm(20),ncol=2)
y <- sample(0:1,10,TRUE)
## no bias reduction
glpls1a(x,y,br=FALSE)

## no bias reduction and 1 PLS component
glpls1a(x,y,K.prov=1,br=FALSE)

## bias reduction
glpls1a(x,y,br=TRUE)
```

glpls1a.cv.error	<i>Leave-one-out cross-validation error using IRWPLS and IRWPLSF model</i>
------------------	--

Description

Leave-one-out cross-validation training set classification error for fitting IRWPLS or IRWPLSF model for two group classification

Usage

```
glpls1a.cv.error(train.X,train.y, K.prov=NULL,eps=1e-3,lmax=100,family="binomial",link="logit",b
```

Arguments

train.X	n by p design matrix (with no intercept term) for training set
train.y	response vector (0 or 1) for training set
K.prov	number of PLS components, default is the rank of train.X
eps	tolerance for convergence
lmax	maximum number of iteration allowed
family	glm family, binomial is the only relevant one here
link	link function, logit is the only one practically implemented now
br	TRUE if Firth's bias reduction procedure is used

Value

error	LOOCV training error
error.obs	the misclassified error observation indices

Author(s)

Beiyong Ding, Robert Gentleman

References

- Ding, B.Y. and Gentleman, R. (2003) *Classification using generalized partial least squares*.
- Marx, B.D (1996) Iteratively reweighted partial least squares estimation for generalized linear regression. *Technometrics* 38(4): 374-381.

See Also

[glpls1a.train.test.error](#), [glpls1a.mlogit.cv.error](#), [glpls1a](#), [glpls1a.mlogit](#), [glpls1a.logit.all](#)

Examples

```
x <- matrix(rnorm(20),ncol=2)
y <- sample(0:1,10,TRUE)

## no bias reduction
glpls1a.cv.error(x,y,br=FALSE)
## bias reduction and 1 PLS component
glpls1a.cv.error(x,y,K.prov=1, br=TRUE)
```

glpls1a.logit.all *Fit MIRWPLS and MIRWPLSF model separately for logits*

Description

Apply Iteratively ReWeighted Least Squares (MIRWPLS) with an option of Firth's bias reduction procedure (MIRWPLSF) for multi-group (say C+1 classes) classification by fitting logit models for all C classes vs baseline class separately.

Usage

```
glpls1a.logit.all(X, y, K.prov = NULL, eps = 0.001, lmax = 100, b.ini = NULL, denom.eps = 1e-20,
```

Arguments

X	n by p design matrix (with no intercept term)
y	response vector with class labels 1 to C+1 for C+1 group classification, baseline class should be 1
K.prov	number of PLS components
eps	tolerance for convergence
lmax	maximum number of iteration allowed
b.ini	initial value of regression coefficients
denom.eps	small quantity to guarantee nonzero denominator in deciding convergence
family	glm family, binomial (i.e. multinomial here) is the only relevant one here
link	link function, logit is the only one practically implemented now
br	TRUE if Firth's bias reduction procedure is used

Value

coefficients regression coefficient matrix

Author(s)

Beiyong Ding, Robert Gentleman

References

- Ding, B.Y. and Gentleman, R. (2003) *Classification using generalized partial least squares*.
- Marx, B.D (1996) Iteratively reweighted partial least squares estimation for generalized linear regression. *Technometrics* 38(4): 374-381.

See Also

[glpls1a.mlogit](#), [glpls1a](#), [glpls1a.mlogit.cv.error](#), [glpls1a.train.test.error](#), [glpls1a.cv.error](#)

Examples

```
x <- matrix(rnorm(20),ncol=2)
y <- sample(1:3,10,TRUE)
## no bias reduction
glpls1a.logit.all(x,y,br=FALSE)
## bias reduction
glpls1a.logit.all(x,y,br=TRUE)
```

glpls1a.mlogit

Fit MIRWPLS and MIRWPLSF model

Description

Fit multi-logit Iteratively ReWeighted Least Squares (MIRWPLS) with an option of Firth's bias reduction procedure (MIRWPLSF) for multi-group classification

Usage

```
glpls1a.mlogit(x, y, K.prov = NULL, eps = 0.001, lmax = 100, b.ini = NULL, denom.eps = 1e-20, fa
```

Arguments

x	n by p design matrix (with intercept term)
y	response vector with class labels 1 to C+1 for C+1 group classification, baseline class should be 1
K.prov	number of PLS components
eps	tolerance for convergence
lmax	maximum number of iteration allowed
b.ini	initial value of regression coefficients
denom.eps	small quantity to guarantee nonzero denominator in deciding convergence
family	glm family, binomial (i.e. multinomial here) is the only relevant one here
link	link function, logit is the only one practically implemented now
br	TRUE if Firth's bias reduction procedure is used

Value

coefficients	regression coefficient matrix
convergence	whether convergence is achieved
niter	total number of iterations
bias.reduction	whether Firth's procedure is used

Author(s)

Beiyong Ding, Robert Gentleman

References

- Ding, B.Y. and Gentleman, R. (2003) *Classification using generalized partial least squares*.
- Marx, B.D (1996) Iteratively reweighted partial least squares estimation for generalized linear regression. *Technometrics* 38(4): 374-381.

See Also

[glpls1a](#), [glpls1a.mlogit.cv.error](#), [glpls1a.train.test.error](#), [glpls1a.cv.error](#)

Examples

```
x <- matrix(rnorm(20), ncol=2)
y <- sample(1:3, 10, TRUE)
## no bias reduction and 1 PLS component
glpls1a.mlogit(cbind(rep(1, 10), x), y, K.prov=1, br=FALSE)
## bias reduction
glpls1a.mlogit(cbind(rep(1, 10), x), y, br=TRUE)
```

glpls1a.mlogit.cv.error

Leave-one-out cross-validation error using MIRWPLS and MIRW-PLSF model

Description

Leave-one-out cross-validation training set error for fitting MIRWPLS or MIRWPLSF model for multi-group classification

Usage

```
glpls1a.mlogit.cv.error(train.X, train.y, K.prov = NULL, eps = 0.001, lmax = 100, mlogit = T, br
```

Arguments

train.X	n by p design matrix (with no intercept term) for training set
train.y	response vector with class labels 1 to C+1 for C+1 group classification, baseline class should be 1
K.prov	number of PLS components
eps	tolerance for convergence
lmax	maximum number of iteration allowed
mlogit	if TRUE use the multinomial logit model, otherwise fit all C-1 logistic models (vs baseline class 1) separately
br	TRUE if Firth's bias reduction procedure is used

Value

error LOOCV training error
 error.obs the misclassified error observation indices

Author(s)

Beiyong Ding, Robert Gentleman

References

- Ding, B.Y. and Gentleman, R. (2003) *Classification using generalized partial least squares*.
- Marx, B.D (1996) Iteratively reweighted partial least squares estimation for generalized linear regression. *Technometrics* 38(4): 374-381.

See Also

[glpls1a.cv.error](#), [glpls1a.train.test.error](#), [glpls1a](#), [glpls1a.mlogit](#), [glpls1a.logit.all](#)

Examples

```
x <- matrix(rnorm(20),ncol=2)
y <- sample(1:3,10,TRUE)

## no bias reduction
glpls1a.mlogit.cv.error(x,y,br=FALSE)
glpls1a.mlogit.cv.error(x,y,mlogit=FALSE,br=FALSE)
## bias reduction
glpls1a.mlogit.cv.error(x,y,br=TRUE)
glpls1a.mlogit.cv.error(x,y,mlogit=FALSE,br=TRUE)
```

glpls1a.train.test.error

out-of-sample test set error using IRWPLS and IRWPLSF model

Description

Out-of-sample test set error for fitting IRWPLS or IRWPLSF model on the training set for two-group classification

Usage

```
glpls1a.train.test.error(train.X,train.y,test.X,test.y,K.prov=NULL,eps=1e-3,lmax=100,family="binomial")
```

Arguments

train.X n by p design matrix (with no intercept term) for training set
 train.y response vector (0 or 1) for training set
 test.X transpose of the design matrix (with no intercept term) for test set
 test.y response vector (0 or 1) for test set

K.prov	number of PLS components, default is the rank of train.X
eps	tolerance for convergence
lmax	maximum number of iteration allowed
family	glm family, binomial is the only relevant one here
link	link function, logit is the only one practically implemented now
br	TRUE if Firth's bias reduction procedure is used

Value

error	out-of-sample test error
error.obs	the misclassified error observation indices
predict.test	the predicted probabilities for test set

Author(s)

Beiyong Ding, Robert Gentleman

References

- Ding, B.Y. and Gentleman, R. (2003) *Classification using generalized partial least squares*.
- Marx, B.D (1996) Iteratively reweighted partial least squares estimation for generalized linear regression. *Technometrics* 38(4): 374-381.

See Also

[glpls1a.cv.error](#), [glpls1a.mlogit.cv.error](#), [glpls1a](#), [glpls1a.mlogit](#), [glpls1a.logit.all](#)

Examples

```
x <- matrix(rnorm(20),ncol=2)
y <- sample(0:1,10,TRUE)
x1 <- matrix(rnorm(10),ncol=2)
y1 <- sample(0:1,5,TRUE)

## no bias reduction
glpls1a.train.test.error(x,y,x1,y1,br=FALSE)
## bias reduction
glpls1a.train.test.error(x,y,x1,y1,br=TRUE)
```

gpls

A function to fit Generalized partial least squares models.

Description

Partial least squares is a commonly used dimension reduction technique. The paradigm can be extended to include generalized linear models in several different ways. The code in this function uses the extension proposed by Ding and Gentleman, 2004.

Usage

```

gpls(x, ...)

## Default S3 method:
gpls(x, y, K.prov=NULL, eps=1e-3, lmax=100, b.ini=NULL,
      denom.eps=1e-20, family="binomial", link=NULL, br=TRUE, ...)

## S3 method for class 'formula'
gpls(formula, data, contrasts=NULL, K.prov=NULL,
      eps=1e-3, lmax=100, b.ini=NULL, denom.eps=1e-20, family="binomial",
      link=NULL, br=TRUE, ...)

```

Arguments

x	The matrix of covariates.
formula	A formula of the form 'y ~ x1 + x2 + ...', where y is the response and the other terms are covariates.
y	The vector of responses
data	A data.frame to resolve the formula, if used
K.prov	number of PLS components, default is the rank of X
eps	tolerance for convergence
lmax	maximum number of iteration allowed
b.ini	initial value of regression coefficients
denom.eps	small quantity to guarantee nonzero denominator in deciding convergence
family	glm family, binomial is the only relevant one here
link	link function, logit is the only one practically implemented now
br	TRUE if Firth's bias reduction procedure is used
...	Additional arguments.
contrasts	an optional list. See the contrasts.arg of model.matrix.default.

Details

This is a different interface to the functionality provided by [gpls1a](#). The interface is intended to be simpler to use and more consistent with other machine learning code in R.

The technology is intended to deal with two class problems where there are more predictors than cases. If a response variable (y) is used that has more than two levels the behavior may be unusual.

Value

An object of class `gpls` with the following components:

coefficients	The estimated coefficients.
convergence	A boolean indicating whether convergence was achieved.
niter	The total number of iterations.
bias.reduction	A boolean indicating whether Firth's procedure was used.
family	The family argument that was passed in.

link	The link argument that was passed in.
terms	The constructed terms object.
call	The call
levs	The factor levels for prediction.

Author(s)

B. Ding and R. Gentleman

References

- Ding, B.Y. and Gentleman, R. (2003) *Classification using generalized partial least squares*.
- Marx, B.D (1996) Iteratively reweighted partial least squares estimation for generalized linear regression. *Technometrics* 38(4): 374-381.

See Also

[glpls1a](#)

Examples

```
library(MASS)
m1 = gpls(type~., data=Pima.tr, K=3)
```

predict.gpls	<i>A prediction method for gpls.</i>
--------------	--------------------------------------

Description

A simple prediction method for gpls objects.

Usage

```
## S3 method for class 'gpls'
predict(object, newdata, ...)
```

Arguments

object	A gpls object, typically obtained from a call to gpls
newdata	New data, for which predictions are desired.
...	Other arguments to be passed on

Details

The prediction method is straight forward. The estimated coefficients from object are used, together with the new data to produce predicted values. These are then split, according to whether the predicted values is larger or smaller than 0.5 and predictions returned.

The code is similar to that in [glpls1a.train.test.error](#) except that in that function both the test and train matrices are centered and scaled (the covariates) by the same values (those from the test data set).

Value

A list of length two:

<code>class</code>	The predicted classes; one for each row of newdata.
<code>predicted</code>	The estimated predictors.

Author(s)

B. Ding and R. Gentleman

See Also

[gpls](#)

Examples

```
example(gpls)
p1 = predict(m1)
```

Index

*Topic **classif**

gpls, 8
predict.gpls, 10

*Topic **regression**

glpls1a, 2
glpls1a.cv.error, 3
glpls1a.logit.all, 4
glpls1a.mlogit, 5
glpls1a.mlogit.cv.error, 6
glpls1a.train.test.error, 7

glpls1a, 2, 4–10
glpls1a.cv.error, 2, 3, 5–8
glpls1a.logit.all, 2, 4, 4, 7, 8
glpls1a.mlogit, 2, 4, 5, 5, 7, 8
glpls1a.mlogit.cv.error, 2, 4–6, 6, 8
glpls1a.train.test.error, 2, 4–7, 7, 10
gpls, 8, 10, 11

predict.gpls-method (predict.gpls), 10
predict.gpls, 10
print.gpls (gpls), 8