

Package ‘pvclass’

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Description Computes nonparametric p-values for the potential class memberships of new observations as well as cross-validated p-values for the training data. The p-values are based on permutation tests applied to an estimated Bayesian likelihood ratio, using a plug-in statistic for the Gaussian model, 'k nearest neighbors', 'weighted nearest neighbors' or 'penalized logistic regression'. Additionally, it provides graphical displays and quantitative analyses of the p-values.

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Author Niki Zumbrennen [aut, cre],
Lutz Duembgen. [aut]

Maintainer Niki Zumbrennen <niki.zumbrennen@gmail.com>

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pvclass-package	<i>P-Values for Classification</i>
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Description

Computes nonparametric p-values for the potential class memberships of new observations as well as cross-validated p-values for the training data. The p-values are based on permutation tests applied to an estimated Bayesian likelihood ratio, using a plug-in statistic for the Gaussian model, 'k nearest neighbors', 'weighted nearest neighbors' or 'penalized logistic regression'.

Additionally, it provides graphical displays and quantitative analyses of the p-values.

Details

Use `cvpvs` to compute cross-validated p-values, `pvs` to classify new observations and `analyze.pvs` to analyze the p-values.

Author(s)

Niki Zumbrennen <niki.zumbrennen@gmail.com>

Lutz Dümbgen <lutz.duembgen@stat.unibe.ch>

https://www.imsv.unibe.ch/about_us/staff/prof_dr_duembgen_lutz/index_eng.html

References

Zumbrennen N. and Dümbgen L. (2017) pvclass: An R Package for p Values for Classification. *Journal of Statistical Software* **78(4)**, 1–19. doi:10.18637/jss.v078.i04

Dümbgen L., Igl B.-W. and Munk A. (2008) P-Values for Classification. *Electronic Journal of Statistics* **2**, 468–493, available at doi:10.1214/08EJS245.

Zumbrennen N. (2014) P-Values for Classification – Computational Aspects and Asymptotics. Ph.D. thesis, University of Bern, available at <http://boris.unibe.ch/id/eprint/53585>.

Examples

```
X <- iris[c(1:49, 51:99, 101:149), 1:4]
```

```
Y <- iris[c(1:49, 51:99, 101:149), 5]
```

```
NewX <- iris[c(50, 100, 150), 1:4]
```

```
cv <- cvpvs(X,Y)
```

```
analyze.pvs(cv,Y)
```

```
pv <- pvs(NewX, X, Y, method = 'k', k = 10)
analyze.pvs(pv)
```

analyze.pvs

Analyze P-Values

Description

Graphical displays and quantitative analyses of a matrix of p-values.

Usage

```
analyze.pvs(pv, Y = NULL, alpha = 0.05, roc = TRUE, pvplot = TRUE, cex = 1)
```

Arguments

pv	matrix with p-values, e.g. output of <code>cvpvs</code> or <code>pvs</code> .
Y	optional. Vector indicating the classes which the observations belong to.
alpha	test level, i.e. 1 - confidence level.
roc	logical. If TRUE and Y is not NULL, ROC curves are plotted.
pvplot	logical. If TRUE or Y is NULL, the p-values are displayed graphically.
cex	A numerical value giving the amount by which plotting text should be magnified relative to the default.

Details

Displays the p-values graphically, i.e. it plots for each p-value a rectangle. The area of this rectangle is proportional to the p-value. The rectangle is drawn blue if the p-value is greater than alpha and red otherwise.

If Y is not NULL, i.e. the class memberships of the observations are known (e.g. cross-validated p-values), then additionally it plots the empirical ROC curves and prints some empirical conditional inclusion probabilities $I(b, \theta)$ and/or pattern probabilities $P(b, S)$. Precisely, $I(b, \theta)$ is the proportion of training observations of class b whose p-value for class θ is greater than α , while $P(b, S)$ is the proportion of training observations of class b such that the $(1 - \alpha)$ -prediction region equals S .

Value

T	Table containing empirical conditional inclusion and/or pattern probabilities for each class b . In case of $L = 2$ or $L = 3$ classes, all patterns S are considered. In case of $L > 3$, all inclusion probabilities and some special patterns S are considered.
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Niki Zumbrennen <niki.zumbrennen@gmail.com>

Lutz Dümbgen <lutz.duembgen@stat.unibe.ch>

https://www.imsv.unibe.ch/about_us/staff/prof_dr_duembgen_lutz/index_eng.html

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See Also

[cvpvs](#), [pvs](#)

Examples

```
X <- iris[c(1:49, 51:99, 101:149), 1:4]
Y <- iris[c(1:49, 51:99, 101:149), 5]
NewX <- iris[c(50, 100, 150), 1:4]

cv <- cvpvs(X,Y)
analyze.pvs(cv,Y)

pv <- pvs(NewX, X, Y, method = 'k', k = 10)
analyze.pvs(pv)
```

buerk

Medical Dataset

Description

This data set collected by Dr. Bürk at the university hospital in Lübeck contains data of 21556 surgeries in a certain time period (end of the nineties). Besides the mortality and the morbidity it contains 21 variables describing the condition of the patient and the surgery.

Usage

```
data(buerk)
```

Format

A data frame with 21556 observations on the following 23 variables.

age Age in years

sex Sex (1 = female, 0 = male)

asa ASA-Score (American Society of Anesthesiologists), describes the physical condition on an ordinal scale:

1 = A normal healthy patient

2 = A patient with mild systemic disease

3 = A patient with severe systemic disease

4 = A patient with severe systemic disease that is a constant threat to life

5 = A moribund patient who is not expected to survive without the operation

6 = A declared brain-dead patient whose organs are being removed for donor purposes

rf_cer Risk factor: cerebral (1 = yes, 0 = no)

rf_car Risk factor: cardiovascular (1 = yes, 0 = no)

rf_pul Risk factor: pulmonary (1 = yes, 0 = no)

rf_ren Risk factor: renal (1 = yes, 0 = no)

rf_hep Risk factor: hepatic (1 = yes, 0 = no)

rf_imu Risk factor: immunological (1 = yes, 0 = no)

rf_metab Risk factor: metabolic (1 = yes, 0 = no)

rf_noc Risk factor: uncooperative, unreliable (1 = yes, 0 = no)

e_malig Etiology: malignant (1 = yes, 0 = no)

e_vascu Etiology: vascular (1 = yes, 0 = no)

antibio Antibiotics therapy (1 = yes, 0 = no)

op Surgery indicated (1 = yes, 0 = no)

opacute Emergency operation (1 = yes, 0 = no)

optime Surgery time in minutes

opsepsis Septic surgery (1 = yes, 0 = no)

opskill Experienced surgeon, i.e. senior physician (1 = yes, 0 = no)

blood Blood transfusion necessary (1 = yes, 0 = no)

icu Intensive care necessary (1 = yes, 0 = no)

mortal Mortality (1 = yes, 0 = no)

morb Morbidity (1 = yes, 0 = no)

Source

Dümbgen L., Igl B.-W. and Munk A. (2008) P-Values for Classification. *Electronic Journal of Statistics* 2, 468–493, available at [doi:10.1214/08EJS245](https://doi.org/10.1214/08EJS245).

References

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 cvpvs

Cross-Validated P-Values

Description

Computes cross-validated nonparametric p-values for the potential class memberships of the training data.

Usage

```
cvpvs(X, Y, method = c('gaussian', 'knn', 'wnn', 'logreg'), ...)
```

Arguments

X	matrix containing training observations, where each observation is a row vector.
Y	vector indicating the classes which the training observations belong to.
method	one of the following methods: 'gaussian': plug-in statistic for the standard Gaussian model, 'knn': k nearest neighbors, 'wnn': weighted nearest neighbors, 'logreg': multicategory logistic regression with l_1 -penalization.
...	further arguments depending on the method (see cvpvs.gaussian , cvpvs.knn , cvpvs.wnn , cvpvs.logreg).

Details

Computes cross-validated nonparametric p-values for the potential class memberships of the training data. Precisely, for each feature vector $X[i,]$ and each class b the number $PV[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

This p-value is based on a permutation test applied to an estimated Bayesian likelihood ratio, using a plug-in statistic for the Gaussian model, 'k nearest neighbors', 'weighted nearest neighbors' or multicategory logistic regression with l_1 -penalization (see [cvpvs.gaussian](#), [cvpvs.knn](#), [cvpvs.wnn](#), [cvpvs.logreg](#)) with estimated prior probabilities $N(b)/n$. Here $N(b)$ is the number of observations of class b and n is the total number of observations.

Value

PV is a matrix containing the cross-validated p-values. Precisely, for each feature vector $X[i,]$ and each class b the number $PV[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

Author(s)

Niki Zumbrunnen <niki.zumbrunnen@gmail.com>

Lutz Dümbgen <lutz.duembgen@stat.unibe.ch>

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See Also

[cvpvs.gaussian](#), [cvpvs.knn](#), [cvpvs.wnn](#), [cvpvs.logreg](#), [pvs](#), [analyze.pvs](#)

Examples

```
X <- iris[,1:4]
Y <- iris[,5]

cvpvs(X,Y,method='k',k=10,distance='d')
```

cvpvs.gaussian

Cross-Validated P-Values (Gaussian)

Description

Computes cross-validated nonparametric p-values for the potential class memberships of the training data. The p-values are based on a plug-in statistic for the standard Gaussian model. The latter means that the conditional distribution of X , given $Y = y$, is Gaussian with mean depending on y and a global covariance matrix.

Usage

```
cvpvs.gaussian(X, Y, cova = c('standard', 'M', 'sym'))
```

Arguments

X	matrix containing training observations, where each observation is a row vector.
Y	vector indicating the classes which the training observations belong to.
cova	estimator for the covariance matrix: 'standard': standard estimator, 'M': M-estimator, 'sym': symmetrized M-estimator.

Details

Computes cross-validated nonparametric p-values for the potential class memberships of the training data. Precisely, for each feature vector $X[i,]$ and each class b the number $PV[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

This p-value is based on a permutation test applied to an estimated Bayesian likelihood ratio, using a plug-in statistic for the standard Gaussian model with estimated prior probabilities $N(b)/n$. Here $N(b)$ is the number of observations of class b and n is the total number of observations.

Value

PV is a matrix containing the cross-validated p-values. Precisely, for each feature vector $X[i,]$ and each class b the number $PV[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

Author(s)

Niki Zumbrennen <niki.zumbrennen@gmail.com>

Lutz Dümbgen <lutz.duembgen@stat.unibe.ch>

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References

Zumbrennen N. and Dümbgen L. (2017) pvclass: An R Package for p Values for Classification. *Journal of Statistical Software* **78(4)**, 1–19. doi:10.18637/jss.v078.i04

Dümbgen L., Igl B.-W. and Munk A. (2008) P-Values for Classification. *Electronic Journal of Statistics* **2**, 468–493, available at doi:10.1214/08EJS245.

Zumbrennen N. (2014) P-Values for Classification – Computational Aspects and Asymptotics. Ph.D. thesis, University of Bern, available at <http://boris.unibe.ch/id/eprint/53585>.

See Also

[cvpvs](#), [cvpvs.knn](#), [cvpvs.wnn](#), [cvpvs.logreg](#)

Examples

```
X <- iris[, 1:4]
```

```
Y <- iris[, 5]
```

```
cvpvs.gaussian(X, Y, cova = 'standard')
```

 cvpvs.knn

Cross-Validated P-Values (k Nearest Neighbors)

Description

Computes cross-validated nonparametric p-values for the potential class memberships of the training data. The p-values are based on 'k nearest neighbors'.

Usage

```
cvpvs.knn(X, Y, k = NULL, distance = c('euclidean', 'ddeuclidean',
    'mahalanobis'), cova = c('standard', 'M', 'sym'))
```

Arguments

X	matrix containing training observations, where each observation is a row vector.
Y	vector indicating the classes which the training observations belong to.
k	number of nearest neighbors. If k is a vector or k = NULL, the program searches for the best k. For more information see section 'Details'.
distance	the distance measure: "euclidean": fixed Euclidean distance, "ddeuclidean": data driven Euclidean distance (component-wise standardization), "mahalanobis": Mahalanobis distance.
cova	estimator for the covariance matrix: 'standard': standard estimator, 'M': M-estimator, 'sym': symmetrized M-estimator.

Details

Computes cross-validated nonparametric p-values for the potential class memberships of the training data. Precisely, for each feature vector $X[i,]$ and each class b the number $PV[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

This p-value is based on a permutation test applied to an estimated Bayesian likelihood ratio, using 'k nearest neighbors' with estimated prior probabilities $N(b)/n$. Here $N(b)$ is the number of observations of class b and n is the total number of observations.

If k is a vector, the program searches for the best k . To determine the best k for the p-value $PV[i, b]$, the class label of the training observation $X[i,]$ is set temporarily to b and then for all training observations with $Y[j] \neq b$ the proportion of the k nearest neighbors of $X[j,]$ belonging to class b is computed. Then the k which minimizes the sum of these values is chosen.

If $k = \text{NULL}$, it is set to $2:\text{ceiling}(\text{length}(Y)/2)$.

Value

PV is a matrix containing the cross-validated p-values. Precisely, for each feature vector $X[i,]$ and each class b the number $PV[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

If k is a vector or NULL, PV has an attribute "opt.k", which is a matrix and $\text{opt.k}[i, b]$ is the best k for observation $X[i,]$ and class b (see section 'Details'). $\text{opt.k}[i, b]$ is used to compute the p-value for observation $X[i,]$ and class b .

Author(s)

Niki Zumbrunnen <niki.zumbrunnen@gmail.com>

Lutz Dümbgen <lutz.duembgen@stat.unibe.ch>

https://www.imsv.unibe.ch/about_us/staff/prof_dr_duembgen_lutz/index_eng.html

References

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Zumbrunnen N. (2014) P-Values for Classification – Computational Aspects and Asymptotics. Ph.D. thesis, University of Bern, available at <http://boris.unibe.ch/id/eprint/53585>.

See Also

[cvpvs](#), [cvpvs.gaussian](#), [cvpvs.wnn](#), [cvpvs.logreg](#)

Examples

```
X <- iris[, 1:4]
Y <- iris[, 5]

cvpvs.knn(X, Y, k = c(5, 10, 15))
```

cvpvs.logreg	<i>Cross-Validated P-Values (Penalized Multicategory Logistic Regression)</i>
--------------	---

Description

Computes cross-validated nonparametric p-values for the potential class memberships of the training data. The p-values are based on 'penalized logistic regression'.

Usage

```
cvpvs.logreg(X, Y, tau.o=10, find.tau=FALSE, delta=2, tau.max=80, tau.min=1,
  pen.method = c("vectors", "simple", "none"), progress = TRUE)
```

Arguments

X	matrix containing training observations, where each observation is a row vector.
Y	vector indicating the classes which the training observations belong to.
tau.o	the penalty parameter (see section 'Details' below).
find.tau	logical. If TRUE the program searches for the best tau. For more information see section 'Details'.
delta	factor for the penalty parameter. Should be greater than 1. Only needed if find.tau == TRUE.
tau.max	maximal penalty parameter considered. Only needed if find.tau == TRUE.
tau.min	minimal penalty parameter considered. Only needed if find.tau == TRUE.
pen.method	the method of penalization (see section 'Details' below).
progress	optional parameter for reporting the status of the computations.

Details

Computes cross-validated nonparametric p-values for the potential class memberships of the training data. Precisely, for each feature vector $X[i,]$ and each class b the number $PV[i, b]$ is a p-value for the null hypothesis that $Y[i]$ equals b , based on the remaining training observations.

This p-value is based on a permutation test applied to an estimated Bayesian likelihood ratio, using 'penalized logistic regression'. This means, the conditional probability of $Y = y$, given $X = x$, is assumed to be proportional to $\exp(a_y + b_y^T x)$. The parameters a_y, b_y are estimated via penalized maximum log-likelihood. The penalization is either a weighted sum of the euclidean norms of the vectors $(b_1[j], b_2[j], \dots, b_L[j])$ (`pen.method=='vectors'`) or a weighted sum of all moduli $|b_y[j]|$ (`pen.method=='simple'`). The weights are given by `tau.o` times the sample standard deviation (within groups) of the j -th components of the feature vectors. In case of `pen.method=='none'`, no penalization is used, but this option may be unstable.

If `find.tau == TRUE`, the program searches for the best penalty parameter. To determine the best parameter `tau` for the p-value $PV[i, b]$, the class label of the training observation $X[i,]$ is set temporarily to b and then for all training observations with $Y[j] \neq b$ the estimated probability of $X[j,]$ belonging to class b is computed. Then the `tau` which minimizes the sum of these values is chosen. First, `tau.o` is compared with `tau.o*delta`. If `tau.o*delta` is better, it is compared with `tau.o*delta^2`, etc. The maximal parameter considered is `tau.max`. If `tau.o` is better than `tau.o*delta`, it is compared with `tau.o*delta^-1`, etc. The minimal parameter considered is `tau.min`.

Value

`PV` is a matrix containing the cross-validated p-values. Precisely, for each feature vector $X[i,]$ and each class b the number $PV[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$, based on the remaining training observations.

If `find.tau == TRUE`, `PV` has an attribute "`tau.opt`", which is a matrix and `tau.opt[i, b]` is the best `tau` for observation $X[i,]$ and class b (see section 'Details'). `tau.opt[i, b]` is used to compute the p-value for observation $X[i,]$ and class b .

Author(s)

Niki Zumbrunnen <niki.zumbrunnen@gmail.com>

Lutz Dümbgen <lutz.duembgen@stat.unibe.ch>

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References

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See Also

[cvpvs](#), [cvpvs.gaussian](#), [cvpvs.knn](#), [cvpvs.wnn](#)

Examples

```

## Not run:
X <- iris[, 1:4]
Y <- iris[, 5]

cvpvs.logreg(X, Y, tau.o=1, pen.method="vectors",progress=TRUE)

## End(Not run)

# A bigger data example: Buerk's hospital data.
## Not run:
data(buerk)
X.raw <- as.matrix(buerk[,1:21])
Y.raw <- buerk[,22]
n0.raw <- sum(1 - Y.raw)
n1 <- sum(Y.raw)
n0 <- 3*n1

X0 <- X.raw[Y.raw==0,]
X1 <- X.raw[Y.raw==1,]

tmpi0 <- sample(1:n0.raw,size=n0,replace=FALSE)
tmpi1 <- sample(1:n1      ,size=n1,replace=FALSE)

X <- rbind(X0[tmpi0,],X1)
Y <- c(rep(1,n0),rep(2,n1))

str(X)
str(Y)

PV <- cvpvs.logreg(X,Y,
tau.o=5,pen.method="v",progress=TRUE)

analyze.pvs(Y=Y,pv=PV,pvplot=FALSE)

## End(Not run)

```

cvpvs.wnn

Cross-Validated P-Values (Weighted Nearest Neighbors)

Description

Computes cross-validated nonparametric p-values for the potential class memberships of the training data. The p-values are based on 'weighted nearest-neighbors'.

Usage

```

cvpvs.wnn(X, Y, wtype = c('linear', 'exponential'), W = NULL,
tau = 0.3, distance = c('euclidean', 'ddeuclidean',
'mahalanobis'), cova = c('standard', 'M', 'sym'))

```

Arguments

X	matrix containing training observations, where each observation is a row vector.
Y	vector indicating the classes which the training observations belong to.
wtype	type of the weight function (see section 'Details' below).
W	vector of the (decreasing) weights (see section 'Details' below).
tau	parameter of the weight function. If tau is a vector or tau = NULL, the program searches for the best tau. For more information see section 'Details'.
distance	the distance measure: "euclidean": fixed Euclidean distance, "ddeuclidean": data driven Euclidean distance (component-wise standardization), "mahalanobis": Mahalanobis distance.
cova	estimator for the covariance matrix: 'standard': standard estimator, 'M': M-estimator, 'sym': symmetrized M-estimator.

Details

Computes cross-validated nonparametric p-values for the potential class memberships of the training data. Precisely, for each feature vector $X[i,]$ and each class b the number $PV[i, b]$ is a p-value for the null hypothesis that $Y[i]$ equals b .

This p-value is based on a permutation test applied to an estimated Bayesian likelihood ratio, using 'weighted nearest neighbors' with estimated prior probabilities $N(b)/n$. Here $N(b)$ is the number of observations of class b and n is the total number of observations.

The (decreasing) weights for the observations can be either indicated with a n dimensional vector W or (if $W = \text{NULL}$) one of the following weight functions can be used:

linear:

$$W_i = \max(1 - \frac{i}{n}/\tau, 0),$$

exponential:

$$W_i = (1 - \frac{i}{n})^\tau.$$

If tau is a vector, the program searches for the best tau. To determine the best tau for the p-value $PV[i, b]$, the class label of the training observation $X[i,]$ is set temporarily to b and then for all training observations with $Y[j] \neq b$ the sum of the weights of the observations belonging to class b is computed. Then the tau which minimizes the sum of these values is chosen.

If $W = \text{NULL}$ and $\text{tau} = \text{NULL}$, tau is set to $\text{seq}(0.1, 0.9, 0.1)$ if $\text{wtype} = "l"$ and to $c(1, 5, 10, 20)$ if $\text{wtype} = "e"$.

Value

PV is a matrix containing the cross-validated p-values. Precisely, for each feature vector $X[i,]$ and each class b the number $PV[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

If tau is a vector or NULL (and $W = \text{NULL}$), PV has an attribute "opt.tau", which is a matrix and $\text{opt.tau}[i, b]$ is the best tau for observation $X[i,]$ and class b (see section 'Details'). "opt.tau" is used to compute the p-values.

Author(s)

Niki Zumbrennen <niki.zumbrennen@gmail.com>
 Lutz Dümbgen <lutz.duembgen@stat.unibe.ch>
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See Also

[cvpvs](#), [cvpvs.gaussian](#), [cvpvs.knn](#), [cvpvs.logreg](#)

Examples

```
X <- iris[, 1:4]
Y <- iris[, 5]

cvpvs.wnn(X, Y, wtype = 'l', tau = 0.5)
```

 pvs

P-Values to Classify New Observations

Description

Computes nonparametric p-values for the potential class memberships of new observations.

Usage

```
pvs(NewX, X, Y, method = c('gaussian', 'knn', 'wnn', 'logreg'), ...)
```

Arguments

NewX	data matrix consisting of one or several new observations (row vectors) to be classified.
X	matrix containing training observations, where each observation is a row vector.
Y	vector indicating the classes which the training observations belong to.
method	one of the following methods: 'gaussian': plug-in statistic for the standard Gaussian model, 'knn': k nearest neighbors, 'wnn': weighted nearest neighbors, 'logreg': multicategory logistic regression with l_1 -penalization.

... further arguments depending on the method (see [pvs.gaussian](#), [pvs.knn](#), [pvs.wnn](#), [pvs.logreg](#)).

Details

Computes nonparametric p-values for the potential class memberships of new observations. Precisely, for each new observation $\text{NewX}[i,]$ and each class b the number $\text{PV}[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

This p-value is based on a permutation test applied to an estimated Bayesian likelihood ratio, using a plug-in statistic for the Gaussian model, 'k nearest neighbors', 'weighted nearest neighbors' or multcategory logistic regression with l_1 -penalization (see [pvs.gaussian](#), [pvs.knn](#), [pvs.wnn](#), [pvs.logreg](#)) with estimated prior probabilities $N(b)/n$. Here $N(b)$ is the number of observations of class b and n is the total number of observations.

Value

PV is a matrix containing the p-values. Precisely, for each new observation $\text{NewX}[i,]$ and each class b the number $\text{PV}[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

Author(s)

Niki Zumbrunnen <niki.zumbrunnen@gmail.com>

Lutz Dümbgen <lutz.duembgen@stat.unibe.ch>

https://www.imsv.unibe.ch/about_us/staff/prof_dr_duembgen_lutz/index_eng.html

References

Zumbrunnen N. and Dümbgen L. (2017) pvclass: An R Package for p Values for Classification. *Journal of Statistical Software* **78(4)**, 1–19. doi:10.18637/jss.v078.i04

Dümbgen L., Igl B.-W. and Munk A. (2008) P-Values for Classification. *Electronic Journal of Statistics* **2**, 468–493, available at doi:10.1214/08EJS245.

Zumbrunnen N. (2014) P-Values for Classification – Computational Aspects and Asymptotics. Ph.D. thesis, University of Bern, available at <http://boris.unibe.ch/id/eprint/53585>.

See Also

[pvs.gaussian](#), [pvs.knn](#), [pvs.wnn](#), [pvs.logreg](#), [cvpvs](#), [analyze.pvs](#)

Examples

```
X <- iris[c(1:49, 51:99, 101:149), 1:4]
Y <- iris[c(1:49, 51:99, 101:149), 5]
NewX <- iris[c(50, 100, 150), 1:4]

pvs(NewX, X, Y, method = 'k', k = 10)
```

pvs.gaussian

*P-Values to Classify New Observations (Gaussian)***Description**

Computes nonparametric p-values for the potential class memberships of new observations. The p-values are based on a plug-in statistic for the standard Gaussian model. The latter means that the conditional distribution of X , given $Y = y$, is Gaussian with mean depending on y and a global covariance matrix.

Usage

```
pvs.gaussian(NewX, X, Y, cova = c('standard', 'M', 'sym'))
```

Arguments

NewX	data matrix consisting of one or several new observations (row vectors) to be classified.
X	matrix containing training observations, where each observation is a row vector.
Y	vector indicating the classes which the training observations belong to.
cova	estimator for the covariance matrix: 'standard': standard estimator, 'M': M-estimator, 'sym': symmetrized M-estimator.

Details

Computes nonparametric p-values for the potential class memberships of new observations. Precisely, for each new observation $\text{NewX}[i,]$ and each class b the number $PV[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

This p-value is based on a permutation test applied to an estimated Bayesian likelihood ratio, using a plug-in statistic for the standard Gaussian model with estimated prior probabilities $N(b)/n$. Here $N(b)$ is the number of observations of class b and n is the total number of observations.

Value

PV is a matrix containing the p-values. Precisely, for each new observation $\text{NewX}[i,]$ and each class b the number $PV[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

Author(s)

Niki Zumbrunnen <niki.zumbrunnen@gmail.com>

Lutz Dümbgen <lutz.duembgen@stat.unibe.ch>

https://www.imsv.unibe.ch/about_us/staff/prof_dr_duembgen_lutz/index_eng.html

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- Zumbrunnen N. and Dümmbgen L. (2017) pvclass: An R Package for p Values for Classification. *Journal of Statistical Software* **78(4)**, 1–19. doi:10.18637/jss.v078.i04
- Dümmbgen L., Igl B.-W. and Munk A. (2008) P-Values for Classification. *Electronic Journal of Statistics* **2**, 468–493, available at doi:10.1214/08EJS245.
- Zumbrunnen N. (2014) P-Values for Classification – Computational Aspects and Asymptotics. Ph.D. thesis, University of Bern, available at <http://boris.unibe.ch/id/eprint/53585>.

See Also

[pvs](#), [pvs.knn](#), [pvs.wnn](#), [pvs.logreg](#)

Examples

```
X <- iris[c(1:49, 51:99, 101:149), 1:4]
Y <- iris[c(1:49, 51:99, 101:149), 5]
NewX <- iris[c(50, 100, 150), 1:4]

pvs.gaussian(NewX, X, Y, cova = 'standard')
```

pvs.knn

P-Values to Classify New Observations (k Nearest Neighbors)

Description

Computes nonparametric p-values for the potential class memberships of new observations. The p-values are based on 'k nearest neighbors'.

Usage

```
pvs.knn(NewX, X, Y, k = NULL, distance = c('euclidean', 'ddeuclidean',
    'mahalanobis'), cova = c('standard', 'M', 'sym'))
```

Arguments

NewX	data matrix consisting of one or several new observations (row vectors) to be classified.
X	matrix containing training observations, where each observation is a row vector.
Y	vector indicating the classes which the training observations belong to.
k	number of nearest neighbors. If k is a vector or k = NULL, the program searches for the best k. For more information see section 'Details'.
distance	the distance measure: 'euclidean': fixed Euclidean distance, 'ddeuclidean': data driven Euclidean distance (component-wise standardization), 'mahalanobis': Mahalanobis distance.

cova estimator for the covariance matrix:
 'standard': standard estimator,
 'M': M-estimator,
 'sym': symmetrized M-estimator.

Details

Computes nonparametric p-values for the potential class memberships of new observations. Precisely, for each new observation $\text{NewX}[i,]$ and each class b the number $\text{PV}[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

This p-value is based on a permutation test applied to an estimated Bayesian likelihood ratio, using 'k nearest neighbors' with estimated prior probabilities $N(b)/n$. Here $N(b)$ is the number of observations of class b and n is the total number of observations.

If k is a vector, the program searches for the best k . To determine the best k for the p-value $\text{PV}[i, b]$, the new observation $\text{NewX}[i,]$ is added to the training data with class label b and then for all training observations with $Y[j] \neq b$ the proportion of the k nearest neighbors of $X[j,]$ belonging to class b is computed. Then the k which minimizes the sum of these values is chosen.

If $k = \text{NULL}$, it is set to $2:\text{ceiling}(\text{length}(Y)/2)$.

Value

PV is a matrix containing the p-values. Precisely, for each new observation $\text{NewX}[i,]$ and each class b the number $\text{PV}[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

If k is a vector or NULL , PV has an attribute "opt.k", which is a matrix and $\text{opt.k}[i, b]$ is the best k for observation $\text{NewX}[i,]$ and class b (see section 'Details'). $\text{opt.k}[i, b]$ is used to compute the p-value for observation $\text{NewX}[i,]$ and class b .

Author(s)

Niki Zumbrennen <niki.zumbrennen@gmail.com>

Lutz Dümbgen <lutz.duembgen@stat.unibe.ch>

https://www.imsv.unibe.ch/about_us/staff/prof_dr_duembgen_lutz/index_eng.html

References

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Dümbgen L., Igl B.-W. and Munk A. (2008) P-Values for Classification. *Electronic Journal of Statistics* **2**, 468–493, available at doi:10.1214/08EJS245.

Zumbrennen N. (2014) P-Values for Classification – Computational Aspects and Asymptotics. Ph.D. thesis, University of Bern, available at <http://boris.unibe.ch/id/eprint/53585>.

See Also

[pvs](#), [pvs.gaussian](#), [pvs.wnn](#), [pvs.logreg](#)

Examples

```
X <- iris[c(1:49, 51:99, 101:149), 1:4]
Y <- iris[c(1:49, 51:99, 101:149), 5]
NewX <- iris[c(50, 100, 150), 1:4]

pvs.knn(NewX, X, Y, k = c(5, 10, 15))
```

pvs.logreg	<i>P-Values to Classify New Observations (Penalized Multicategory Logistic Regression)</i>
------------	--

Description

Computes nonparametric p-values for the potential class memberships of new observations. The p-values are based on 'penalized logistic regression'.

Usage

```
pvs.logreg(NewX, X, Y, tau.o = 10, find.tau=FALSE, delta=2, tau.max=80, tau.min=1,
           a0 = NULL, b0 = NULL,
           pen.method = c('vectors', 'simple', 'none'),
           progress = FALSE)
```

Arguments

NewX	data matrix consisting of one or several new observations (row vectors) to be classified.
X	matrix containing training observations, where each observation is a row vector.
Y	vector indicating the classes which the training observations belong to.
tau.o	the penalty parameter (see section 'Details' below).
find.tau	logical. If TRUE the program searches for the best tau. For more information see section 'Details'.
delta	factor for the penalty parameter. Should be greater than 1. Only needed if find.tau == TRUE.
tau.max	maximal penalty parameter considered. Only needed if find.tau == TRUE.
tau.min	minimal penalty parameter considered. Only needed if find.tau == TRUE.
a0, b0	optional starting values for logistic regression.
pen.method	the method of penalization (see section 'Details' below).
progress	optional parameter for reporting the status of the computations.

Details

Computes nonparametric p-values for the potential class memberships of new observations. Precisely, for each new observation $\text{NewX}[i,]$ and each class b the number $\text{PV}[i, b]$ is a p-value for the null hypothesis that $Y[i]$ equals b .

This p-value is based on a permutation test applied to an estimated Bayesian likelihood ratio, using 'penalized logistic regression'. This means, the conditional probability of $Y = y$, given $X = x$, is assumed to be proportional to $\exp(a_y + b_y^T x)$. The parameters a_y, b_y are estimated via penalized maximum log-likelihood. The penalization is either a weighted sum of the euclidean norms of the vectors $(b_1[j], b_2[j], \dots, b_L[j])$ (`pen.method=='vectors'`) or a weighted sum of all moduli $|b_\theta[j]|$ (`pen.method=='simple'`). The weights are given by `tau.o` times the sample standard deviation (within groups) of the j -th components of the feature vectors. In case of `pen.method=='none'`, no penalization is used, but this option may be unstable.

If `find.tau == TRUE`, the program searches for the best penalty parameter. To determine the best parameter τ for the p-value $\text{PV}[i, b]$, the new observation $\text{NewX}[i,]$ is added to the training data with class label b and then for all training observations with $Y[j] \neq b$ the estimated probability of $X[j,]$ belonging to class b is computed. Then the τ which minimizes the sum of these values is chosen. First, `tau.o` is compared with `tau.o*delta`. If `tau.o*delta` is better, it is compared with `tau.o*delta^2`, etc. The maximal parameter considered is `tau.max`. If `tau.o` is better than `tau.o*delta`, it is compared with `tau.o*delta^-1`, etc. The minimal parameter considered is `tau.min`.

Value

PV is a matrix containing the p-values. Precisely, for each new observation $\text{NewX}[i,]$ and each class b the number $\text{PV}[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

If `find.tau == TRUE`, PV has an attribute "tau.opt", which is a matrix and `tau.opt[i, b]` is the best τ for observation $\text{NewX}[i,]$ and class b (see section 'Details'). `tau.opt[i, b]` is used to compute the p-value for observation $\text{NewX}[i,]$ and class b .

Author(s)

Niki Zumbrennen <niki.zumbrennen@gmail.com>

Lutz Dümbgen <lutz.duembgen@stat.unibe.ch>

https://www.imsv.unibe.ch/about_us/staff/prof_dr_duembgen_lutz/index_eng.html

References

Zumbrennen N. and Dümbgen L. (2017) pvclass: An R Package for p Values for Classification. *Journal of Statistical Software* **78(4)**, 1–19. doi:10.18637/jss.v078.i04

Dümbgen L., Igl B.-W. and Munk A. (2008) P-Values for Classification. *Electronic Journal of Statistics* **2**, 468–493, available at doi:10.1214/08EJS245.

Zumbrennen N. (2014) P-Values for Classification – Computational Aspects and Asymptotics. Ph.D. thesis, University of Bern, available at <http://boris.unibe.ch/id/eprint/53585>.

See Also

[pvs](#), [pvs.gaussian](#), [pvs.knn](#), [pvs.wnn](#)

Examples

```

X <- iris[c(1:49, 51:99, 101:149), 1:4]
Y <- iris[c(1:49, 51:99, 101:149), 5]
NewX <- iris[c(50, 100, 150), 1:4]

pvs.logreg(NewX, X, Y, tau.o=1, pen.method="vectors", progress=TRUE)

# A bigger data example: Buerk's hospital data.
## Not run:
data(buerk)
X.raw <- as.matrix(buerk[,1:21])
Y.raw <- buerk[,22]
n0.raw <- sum(1 - Y.raw)
n1 <- sum(Y.raw)
n0 <- 3*n1

X0 <- X.raw[Y.raw==0,]
X1 <- X.raw[Y.raw==1,]

tmpi0 <- sample(1:n0.raw,size=3*n1,replace=FALSE)
tmpi1 <- sample(1:n1 ,size= n1,replace=FALSE)

Xtrain <- rbind(X0[tmpi0[1:(n0-100)],],X1[1:(n1-100),])
Ytrain <- c(rep(1,n0-100),rep(2,n1-100))
Xtest <- rbind(X0[tmpi0[(n0-99):n0],],X1[(n1-99):n1,])
Ytest <- c(rep(1,100),rep(2,100))

PV <- pvs.logreg(Xtest,Xtrain,Ytrain,tau.o=2,progress=TRUE)
analyze.pvs(Y=Ytest,pv=PV,pvplot=FALSE)

## End(Not run)

```

pvs.wnn

P-Values to Classify New Observations (Weighted Nearest Neighbors)

Description

Computes nonparametric p-values for the potential class memberships of new observations. The p-values are based on 'weighted nearest-neighbors'.

Usage

```

pvs.wnn(NewX, X, Y, wtype = c('linear', 'exponential'), W = NULL,
        tau = 0.3, distance = c('euclidean', 'ddeuclidean',
        'mahalanobis'), cova = c('standard', 'M', 'sym'))

```

Arguments

NewX	data matrix consisting of one or several new observations (row vectors) to be classified.
X	matrix containing training observations, where each observation is a row vector.
Y	vector indicating the classes which the training observations belong to.
wtype	type of the weight function (see section 'Details' below).
W	vector of the (decreasing) weights (see section 'Details' below).
tau	parameter of the weight function. If tau is a vector or tau = NULL, the program searches for the best tau. For more information see section 'Details'.
distance	the distance measure: 'euclidean': fixed Euclidean distance, 'd euclidean': data driven Euclidean distance (component-wise standardization), 'mahalanobis': Mahalanobis distance.
cova	estimator for the covariance matrix: 'standard': standard estimator, 'M': M-estimator, 'sym': symmetrized M-estimator.

Details

Computes nonparametric p-values for the potential class memberships of new observations. Precisely, for each new observation $\text{NewX}[i,]$ and each class b the number $\text{PV}[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

This p-value is based on a permutation test applied to an estimated Bayesian likelihood ratio, using 'weighted nearest neighbors' with estimated prior probabilities $N(b)/n$. Here $N(b)$ is the number of observations of class b and n is the total number of observations.

The (decreasing) weights for the observation can be either indicated with a n dimensional vector W or (if $W = \text{NULL}$) one of the following weight functions can be used:

linear:

$$W_i = \max\left(1 - \frac{i}{n}/\tau, 0\right),$$

exponential:

$$W_i = \left(1 - \frac{i}{n}\right)^\tau.$$

If tau is a vector, the program searches for the best tau. To determine the best tau for the p-value $\text{PV}[i, b]$, the new observation $\text{NewX}[i,]$ is added to the training data with class label b and then for all training observations with $Y[j] \neq b$ the sum of the weights of the observations belonging to class b is computed. Then the tau which minimizes the sum of these values is chosen.

If tau = NULL, it is set to $\text{seq}(0.1, 0.9, 0.1)$ if wtype = "l" and to $c(1, 5, 10, 20)$ if wtype = "e".

Value

PV is a matrix containing the p-values. Precisely, for each new observation $\text{NewX}[i,]$ and each class b the number $\text{PV}[i, b]$ is a p-value for the null hypothesis that $Y[i] = b$.

If tau is a vector or NULL (and $W = \text{NULL}$), PV has an attribute "opt.tau", which is a matrix and $\text{opt.tau}[i, b]$ is the best tau for observation $\text{NewX}[i,]$ and class b (see section 'Details'). $\text{opt.tau}[i, b]$ is used to compute the p-value for observation $\text{NewX}[i,]$ and class b .

Author(s)

Niki Zumbrunnen <niki.zumbrunnen@gmail.com>

Lutz Dümbgen <lutz.duembgen@stat.unibe.ch>

https://www.imsv.unibe.ch/about_us/staff/prof_dr_duembgen_lutz/index_eng.html

References

Zumbrunnen N. and Dümbgen L. (2017) pvclass: An R Package for p Values for Classification. *Journal of Statistical Software* **78(4)**, 1–19. doi:10.18637/jss.v078.i04

Dümbgen L., Igl B.-W. and Munk A. (2008) P-Values for Classification. *Electronic Journal of Statistics* **2**, 468–493, available at doi:10.1214/08EJS245.

Zumbrunnen N. (2014) P-Values for Classification – Computational Aspects and Asymptotics. Ph.D. thesis, University of Bern, available at <http://boris.unibe.ch/id/eprint/53585>.

See Also

[pvs](#), [pvs.gaussian](#), [pvs.knn](#), [pvs.logreg](#)

Examples

```
X <- iris[c(1:49, 51:99, 101:149), 1:4]
```

```
Y <- iris[c(1:49, 51:99, 101:149), 5]
```

```
NewX <- iris[c(50, 100, 150), 1:4]
```

```
pvs.wnn(NewX, X, Y, wtype = 'l', tau = 0.5)
```

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