Package ‘pvclass’

October 14, 2022

Type Package

Title P-Values for Classification

Version 1.4

Date 2017-06-05

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Imports Matrix

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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NeedsCompilation no

Repository CRAN

Date/Publication 2017-06-05 15:13:51 UTC

R topics documented:

pvclass-package *P-Values for Classification*

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.

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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 `http://dx.doi.org/10.1214/08-EJS245`.

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`.

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 `cvpvs` or `pvs`.

`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 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 patters S are considered.

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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` Expirienced surgeond, 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 `http://dx.doi.org/10.1214/08-EJS245`.

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 $l1$-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 $l1$-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 $Y[i] = b$.

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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 $Y[i] = b$.

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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.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] != 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 = NULL`, it is set to 2:ceiling(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 `opt.k[i,b]` is the best `k` for observation `X[i,]` and class `b` (see section 'Details'). `opt.k[i,b]` is used to compute the p-value for observation `X[i,]` and class `b`.

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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` *Cross-Validated P-Values (Penalized Multicategory Logistic Regression)*

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 $(b_1[j], b_2[j], \ldots, b_L[j])$ (`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] != 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`.

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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 = 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] != 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 = NULL` and `tau = NULL`, `tau` is set to `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 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 = NULL`), `PV` has an attribute `"opt.tau"`, which is a matrix and `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.

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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 $l1$-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 `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 Gaussian model, 'k nearest neighbors', 'weighted nearest neighbors' or multicategory logistic regression with $l1$-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 `NewX[i,]` and each class `b` the number `PV[i,b]` is a p-value for the null hypothesis that $Y[i] = b$.

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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 `http://dx.doi.org/10.1214/08-EJS245`.

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 `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 `NewX[i,]` and each class `b` the number `PV[i,b]` is a p-value for the null hypothesis that $Y[i] = b$.

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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 `http://dx.doi.org/10.1214/08-EJS245`.

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 `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 ’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 new observation `NewX[i,]` is added to the training data with class label `b` and then for all training observations with `Y[j] != 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 = NULL`, it is set to 2:ceiling(length(Y)/2).

Value

`PV` is a matrix containing the p-values. Precisely, for each new observation `NewX[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 `opt.k[i,b]` is the best `k` for observation `NewX[i,]` and class `b` (see section ’Details’). `opt.k[i,b]` is used to compute the p-value for observation `NewX[i,]` and class `b`.

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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

`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 *P-Values to Classify New Observations (Penalized Multicategory Logistic Regression)*

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 NewX[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 '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 $(b_1[j], b_2[j], \ldots, b_L[j])$ (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 tau for the p-value PV[i,b], the new observation NewX[i,] is added to the training data with class label b and then for all training observations with Y[j] != 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 p-values. Precisely, for each new observation NewX[i,] and each class b the number 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 tau for observation NewX[i,] and class b (see section 'Details'). tau.opt[i,b] is used to compute the p-value for observation NewX[i,] and class b.

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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

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,
'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 `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 '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 = 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 new observation `NewX[i,]` is added to the training data with class label `b` and then for all training observations with `Y[j] != 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 `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 `NewX[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 = NULL`), `PV` has an attribute `"opt.tau"`, which is a matrix and `opt.tau[i,b]` is the best `tau` for observation `NewX[i,]` and class `b` (see section 'Details'). `opt.tau[i,b]` is used to compute the p-value for observation `NewX[i,]` and class `b`.

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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

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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