Package ‘MKclass’

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MKclass-package

Description


Details

Package: MKclass
Type: Package
Version: 0.4
Date: 2020-10-03
Depends: R(>= 4.0.0)
Imports: stats
Suggests: knitr, rmarkdown, foreach, parallel, doParallel
License: LGPL-3
URL: http://www.stamats.de/

library(MKclass)

Author(s)

Matthias Kohl http://www.stamats.de
Maintainer: Matthias Kohl <matthias.kohl@stamats.de>
AUC

Compute AUC

Description

The function computes AUC.

Usage

AUC(x, y, group, switchAUC = TRUE)

Arguments

- **x**: numeric vector.
- **y**: numeric vector. If missing, group has to be specified.
- **group**: grouping vector or factor.
- **switchAUC**: logical value. Switch AUC; see Details section.

Details

The function computes the area under the receiver operating characteristic curve (AUC under ROC curve).

If \( \text{AUC} < 0.5 \), a warning is printed and \( 1 - \text{AUC} \) is returned. This behaviour can be suppressed by using \( \text{switchAUC} = \text{FALSE} \).

The implementation uses the connection of AUC to the Wilcoxon rank sum test; see Hanley and McNeil (1982).

Value

AUC value.

Author(s)

Matthias Kohl <Matthias.Kohl@stamats.de>

References


Examples

```r
set.seed(13)
x <- rnorm(100)  ## assumed as log2-data
g <- sample(1:2, 100, replace = TRUE)
AUC(x, group = g)
## avoid switching AUC
AUC(x, group = g, switchAUC = FALSE)
```
AUC.test

Description

Performs tests for one and two AUCs.

Usage

AUC.test(pred1, lab1, pred2, lab2, conf.level = 0.95, paired = FALSE)

Arguments

- pred1: numeric vector.
- lab1: grouping vector or factor for pred1.
- pred2: numeric vector.
- lab2: grouping vector or factor for pred2.
- conf.level: confidence level of the interval.
- paired: not yet implemented.

Details

If pred2 and lab2 are missing, the AUC for pred1 and lab1 is tested using the Wilcoxon signed rank test; see wilcox.test.

If pred1 and lab1 as well as pred2 and lab2 are specified, the Hanley and McNeil test (cf. Hanley and McNeil (1982)) is computed.

Value

A list with AUC, SE and confidence interval as well as the corresponding test result.

Author(s)

Matthias Kohl <Matthias.Kohl@stamats.de>

References


See Also

wilcox.test, AUC
confMatrix

Examples

```r
set.seed(13)
x <- rnorm(100)  ## assumed as log2-data
g <- sample(1:2, 100, replace = TRUE)
AUC.test(x, g)
y <- rnorm(100)  ## assumed as log2-data
h <- sample(1:2, 100, replace = TRUE)
AUC.test(x, g, y, h)
```

confMatrix

Compute Confusion Matrix

Description

The function computes the confusion matrix of a binary classification.

Usage

```r
confMatrix(pred, pred.group, truth, namePos, cutoff = 0.5, relative = TRUE)
```

Arguments

- `pred`: numeric values that shall be used for classification; e.g. probabilities to belong to the positive group.
- `pred.group`: vector or factor including the predicted group. If missing, `pred.group` is computed from `pred`, where `pred >= cutoff` is classified as positive.
- `truth`: true grouping vector or factor.
- `namePos`: value representing the positive group.
- `cutoff`: cutoff value used for classification.
- `relative`: logical: absolute and relative values.

Details

The function computes the confusion matrix of a binary classification consisting of the number of true positive (TP), false negative (FN), false positive (FP) and true negative (TN) predictions.

In addition, their relative counterparts true positive rate (TPR), false negative rate (FNR), false positive rate (FPR) and true negative rate (TNR) can be computed.

Value

- `matrix` or list of matrices with respective numbers of true and false predictions.

Author(s)

Matthias Kohl <Matthias.Kohl@stamats.de>
decisionStump

References


Examples

```r
## example from dataset infert
fit <- glm(case ~ spontaneous+induced, data = infert, family = binomial())
pred <- predict(fit, type = "response")

## with group numbers
cnfMatrix(pred, truth = infert$case, namePos = 1)

## with group names
my.case <- factor(infert$case, labels = c("control", "case"))
cnfMatrix(pred, truth = my.case, namePos = "case")

## on the scale of the linear predictors
pred2 <- predict(fit)
cnfMatrix(pred2, truth = infert$case, namePos = 1, cutoff = 0)

## only absolute numbers
confMatrix(pred, truth = infert$case, namePos = 1, relative = FALSE)
```

decisionStump: Compute Decision Stumps

Description

The function computes a decision stump for binary classification also known as 1-level decision tree or 1-rule.

Usage

```r
decisionStump(pred, truth, namePos, perfMeasure = "YJS",
             MAX = TRUE, parallel = FALSE, ncores, delta = 0.01, ...)
```

Arguments

- `pred`: numeric values that shall be used for classification; e.g. probabilities to belong to the positive group.
- `truth`: true grouping vector or factor.
- `namePos`: value representing the positive group.
- `perfMeasure`: a single performance measure computed by function `perfMeasure`.
- `MAX`: logical value. Whether to maximize or minimize the performance measure.
- `parallel`: logical value. If `TRUE` packages `foreach` and `doParallel` are used to parallelize the computations.
`HLgof.test` 7

- ncores: integer value, number of cores that shall be used to parallelize the computations.
- delta: numeric value for setting up grid for optimization; start is minimum of pred-delta, end is maximum of pred+delta.
- ... further arguments passed to function `perfMeasures`.

Details

The function is able to compute a decision stump for various performance measures, all performance measures that are implemented in function `perfMeasures`. Of course, for several of them the computation is not really useful such as sensitivity or specificity where one will get trivial decision rules.

Value

Object of class `decisionStump`.

Author(s)

Matthias Kohl <Matthias.Kohl@stamats.de>

References


Examples

```r
## example from dataset infert
fit <- glm(case ~ spontaneous+induced, data = infert, family = binomial())
pred <- predict(fit, type = "response")
res <- decisionStump(pred, truth = infert$case, namePos = 1)
predict(res, newdata = seq(from = 0, to = 1, by = 0.1))
```

---

`HLgof.test`  
Hosmer-Lemeshow goodness of fit tests.

Description

The function computes Hosmer-Lemeshow goodness of fit tests for C and H statistic as well as the le Cessie-van Houwelingen-Copas-Hosmer unweighted sum of squares test for global goodness of fit.

Usage

```r
HLgof.test(fit, obs, ngr = 10, X, verbose = FALSE)
```
Arguments

- **fit**: numeric vector with fitted probabilities.
- **obs**: numeric vector with observed values.
- **ngr**: number of groups for C and H statistic.
- **X**: covariate(s) for le Cessie-van Houwelingen-Copas-Hosmer global goodness of fit test.
- **verbose**: logical, print intermediate results.

Details

Hosmer-Lemeshow goodness of fit tests are computed; see Lemeshow and Hosmer (1982).

If X is specified, the le Cessie-van Houwelingen-Copas-Hosmer unweighted sum of squares test for global goodness of fit is additionally determined; see Hosmer et al. (1997). A more general version of this test is implemented in function `residuals.lrm` in package `rms`.

Value

A list of test results.

Author(s)

Matthias Kohl <Matthias.Kohl@stamats.de>

References


See Also

`residuals.lrm`

Examples

```r
set.seed(111)
x1 <- factor(sample(1:3, 50, replace = TRUE))
x2 <- rnorm(50)
obs <- sample(c(0,1), 50, replace = TRUE)
fit <- glm(obs ~ x1+x2, family = binomial)
HLgof.test(fit = fitted(fit), obs = obs)
HLgof.test(fit = fitted(fit), obs = obs, X = model.matrix(obs ~ x1+x2))
```
optCutoff

Compute the Optimal Cutoff for Binary Classification

Description

The function computes the optimal cutoff for various performance measures for binary classification.

Usage

optCutoff(pred, truth, namePos, perfMeasure = "YJS", 
          MAX = TRUE, parallel = FALSE, ncores, delta = 0.01, ...)

Arguments

- **pred**: numeric values that shall be used for classification; e.g. probabilities to belong to the positive group.
- **truth**: true grouping vector or factor.
- **namePos**: value representing the positive group.
- **perfMeasure**: a single performance measure computed by function `perfMeasure`.
- **MAX**: logical value. Whether to maximize or minimize the performance measure.
- **parallel**: logical value. If TRUE packages foreach and doParallel are used to parallelize the computations.
- **ncores**: integer value, number of cores that shall be used to parallelize the computations.
- **delta**: numeric value for setting up grid for optimization; start is minimum of pred-delta, end is maximum of pred+delta.
- **...**: further arguments passed to function `perfMeasures`.

Details

The function is able to compute the optimal cutoff for various performance measures, all performance measures that are implemented in function `perfMeasures`. Of course, for several of them the computation is not really useful such as sensitivity or specificity where one will get trivial cutoffs.

Value

Optimal cutoff and value of the optimized performance measure based on a simple grid search.

Author(s)

Matthias Kohl <Matthias.Kohl@stamats.de>
Examples

```r
## example from dataset infert
fit <- glm(case ~ spontaneous+induced, data = infert, family = binomial())
pred <- predict(fit, type = "response")
optCutoff(pred, truth = infert$case, namePos = 1)
```

---

### or2rr

**Transform OR to RR**

**Description**

The function transforms a given odds-ratio (OR) to the respective relative risk (RR).

**Usage**

```r
or2rr(or, p0, p1)
```

**Arguments**

- `or`: numeric vector: OR (odds-ratio).
- `p0`: numeric vector of length 1: incidence of the outcome of interest in the nonexposed group.
- `p1`: numeric vector of length 1: incidence of the outcome of interest in the exposed group.

**Details**

The function transforms a given odds-ratio (OR) to the respective relative risk (RR). It can also be used to transform the limits of confidence intervals.

The formulas can be derived by combining the formulas for RR and OR; see also Zhang and Yu (1998).

**Value**

relative risk.

**Author(s)**

Matthias Kohl <Matthias.Kohl@stamats.de>

**References**

Examples

```r
## We use data from Zhang and Yu (1998)

## OR to RR using OR and p0
or2rr(14.1, 0.05)

## compute p1
or2rr(14.1, 0.05)*0.05

## OR to RR using OR and p1
or2rr(14.1, p1 = 0.426)

## OR and 95% confidence interval
or2rr(c(14.1, 7.8, 27.5), 0.05)

## Logistic OR and 95% confidence interval
logisticOR <- rbind(c(14.1, 7.8, 27.5),
                    c(8.7, 5.5, 14.3),
                    c(27.4, 17.2, 45.8),
                    c(4.5, 2.7, 7.8),
                    c(0.25, 0.17, 0.37),
                    c(0.09, 0.05, 0.14))
colnames(logisticOR) <- c("OR", "2.5\%", "97.5\%")
rownames(logisticOR) <- c("7.4", "4.2", "3.0", "2.0", "0.37", "0.14")
logisticOR

## p0
p0 <- c(0.05, 0.12, 0.32, 0.27, 0.40, 0.40)

## Compute corrected RR
## helper function
or2rr.mat <- function(or, p0){
  res <- matrix(NA, nrow = nrow(or), ncol = ncol(or))
  for(i in seq_len(nrow(or))){
    res[i,] <- or2rr(or[i,], p0[i])
  }
dimnames(res) <- dimnames(or)
  res
}
RR <- or2rr.mat(logisticOR, p0)
round(RR, 2)

## Results are not completely identical to Zhang and Yu (1998)
## what probably is caused by the fact that the logistic OR values
## provided in the table are rounded and are not exact values.
```

pairwise.auc  

Compute pairwise AUCs

Description

The function computes pairwise AUCs.
Usage

    pairwise.auc(x, g)

Arguments

x numeric vector.

g grouping vector or factor

Details

The function computes pairwise areas under the receiver operating characteristic curves (AUC under ROC curves) using function AUC.

The implementation is in certain aspects analogously to pairwise.t.test.

Value

Vector with pairwise AUCs.

Author(s)

Matthias Kohl <Matthias.Kohl@stamats.de>

See Also

AUC, pairwise.t.test

Examples

set.seed(13)
x <- rnorm(100)
g <- factor(sample(1:4, 100, replace = TRUE))
levels(g) <- c("a", "b", "c", "d")
pairwise.auc(x, g)

---

perfMeasures

Compute Performance Measures or Binary Classification

Description

The function computes various performance measures for binary classification.

Usage

    perfMeasures(pred, pred.group, truth, namePos, cutoff = 0.5,
                 weight = 0.5, wACC = weight, wLR = weight,
                 wPV = weight, beta = 1, measures = "all")
Arguments

- **pred**: numeric values that shall be used for classification; e.g. probabilities to belong to the positive group.
- **pred.group**: vector or factor including the predicted group. If missing, `pred.group` is computed from `pred`, where `pred >= cutoff` is classified as positive.
- **truth**: true grouping vector or factor.
- **namePos**: value representing the positive group.
- **cutoff**: cutoff value used for classification.
- **weight**: weight used for computing weighted values. Must be in \([0,1]\).
- **wACC**: weight used for computing the weighted accuracy, where sensitivity is multiplied by \(wACC\) and specificity by \(1-wACC\). Must be in \([0,1]\).
- **wLR**: weight used for computing the weighted likelihood ratio, where PLR is multiplied by \(wLR\) and NLR by \(1-wLR\). Must be in \([0,1]\).
- **wPV**: weight used for computing the weighted predictive value, where PPV is multiplied by \(wPV\) and NPV by \(1-wPV\). Must be in \([0,1]\).
- **beta**: beta coefficient used for computing the F beta score. Must be nonnegative.
- **measures**: character vector giving the measures that shall be computed; see details. Default “all” computes all measures available.

Details

The function `perfMeasures` can be used to compute various performance measures. For computing specific measures, the abbreviation given in parentheses have to be specified in argument `measures`. Single measures can also be computed by respective functions, where their names are identical to the abbreviations given in the parentheses.

The measures are: accuracy (ACC), probability of correct classification (PCC), fraction correct (FC), simple matching coefficient (SMC), Rand (similarity) index (RSI), probability of misclassification (PMC), error rate (ER), fraction incorrect (FIC), sensitivity (SENS), recall (REC), true positive rate (TPR), probability of detection (PD), hit rate (HR), specificity (SPEC), true negative rate (TNR), selectivity (SEL), detection rate (DR), false positive rate (FPR), fall-out (FO), false alarm rate (FAR), probability of false alarm (PFA), false negative rate (FNR), miss rate (MR), false discovery rate (FDR), false omission rate (FOR), prevalence (PREV), positive pre-test probability (PREP), positive pre-test odds (PREO), detection prevalence (DPRE), negative pre-test probability (NPRE), negative pre-test odds (NPREO), no information rate (NIR), weighted accuracy (WACC), balanced accuracy (BACC), (bookmaker) informedness (INF), Youden’s J statistic (YJS), deltap’ (DPp), positive likelihood ratio (PLR), negative likelihood ratio (NLR), weighted likelihood ratio (WLR), balanced likelihood ratio (BLR), diagnostic odds ratio (DOR), positive predictive value (PPV), precision (PREC), (positive) post-test probability (POSTP), (positive) post-test odds (POSTO), Bayes factor G1 (BFG1), negative predictive value (NPV), negative post-test probability (NPOSTP), negative post-test odds (NPOSTO), Bayes factor G0 (BFG0), markedness (MARK), deltap (DP), weighted predictive value (WPV), balanced predictive value (BPV), F1 score (F1S), Dice similarity coefficient (DSC), F beta score (FBS), Jaccard similarity coefficient (JSC), threat score (TS), critical success index (CSI), Matthews’ correlation coefficient (MCC), Pearson’s correlation (r phi) (RPHI), Phi coefficient (PHIC), Cramer’s V (CRV), proportion of positive predictions (PPP), expected accuracy (EACC), Cohen’s kappa coefficient (CKC), mutual information in bits...
(MI2), joint entropy in bits (JE2), variation of information in bits (VI2), Jaccard distance (JD), information quality ratio (INFQR), uncertainty coefficient (UC), entropy coefficient (EC), proficiency (metric) (PROF), deficiency (metric) (DFM), redundancy (RED), symmetric uncertainty (SU), normalized uncertainty (NU).

These performance measures have in common that they require a dichotomization of the computed predictions (classification function). For measuring the performance without dichotomization one can apply function `perfScores`.

The prevalence is the prevalence given by the data. This often is not identical to the prevalence of the population. Hence, it might be better to compute PPV and NPV (and derived measures) by applying function `predValues`, where one can specify the assumed prevalence. This holds in general for all measures that depend on the prevalence.

**Value**

data.frame with names of the performance measures and their respective values.

**Author(s)**

Matthias Kohl <Matthias.Kohl@stamats.de>

**References**


B. Wallace, I. Dahabreh (2012). Class probability estimates are unreliable for imbalanced data (and how to fix them). In *Data Mining* (ICDM), IEEE 12th International Conference on, 695-04.

See Also

confMatrix, predValues, perfScores

Examples

## example from dataset infert
fit <- glm(case ~ spontaneous+induced, data = infert, family = binomial())
pred <- predict(fit, type = "response")

## with group numbers
perfMeasures(pred, truth = infert$case, namePos = 1)

## with group names
my.case <- factor(infert$case, labels = c("control", "case"))
predMeasures(pred, truth = my.case, namePos = "case")

## on the scale of the linear predictors
pred2 <- predict(fit)
predMeasures(pred2, truth = infert$case, namePos = 1, cutoff = 0)

## using weights
predMeasures(pred, truth = infert$case, namePos = 1, weight = 0.3)

## selecting a subset of measures
predMeasures(pred, truth = infert$case, namePos = 1, measures = c("SENS", "SPEC", "BACC", "YJS"))

perfScores
Compute Performance Scores for Binary Classification

Description

The function computes various performance scores for binary classification.

Usage

perfScores(pred, truth, namePos, wBS = 0.5, scores = "all", transform = FALSE)

Arguments

pred numeric values that shall be used for classification; e.g. probabilities to belong to the positive group.
truth true grouping vector or factor.
namePos value representing the positive group.
wBS weight used for computing the weighted Brier score (BS), where positive BS is multiplied by wBS and negative BS by 1-wBS. Must be in [0,1].
scores character vector giving the scores that shall be computed; see details. Default "all" computes all scores available.
transform logical value indicating whether the values in pred should be transformed to [0,1]; see details.

Details

The function perfScores can be used to compute various performance scores. For computing specific scores, the abbreviation given in parentheses have to be specified in argument scores. Single scores can also be computed by respective functions, where their names are identical to the abbreviations given in the parentheses.

The available scores are: area under the ROC curve (AUC), Gini index (GINI), Brier score (BS), positive Brier score (PBS), negative Brier score (NBS), weighted Brier score (WBS), balanced Brier score (BBS).

If the predictions (pred) are not in the interval [0,1], the various Brier scores are not valid. By setting argument transform to TRUE, a simple logistic regression model is fit to the provided data and the predicted values are used for the computations.

Value
data.frame with names of the scores and their respective values.

Author(s)

Matthias Kohl <Matthias.Kohl@stamats.de>

References


See Also

`perfMeasures`
Examples

```r
## example from dataset infert
fit <- glm(case ~ spontaneous + induced, data = infert, family = binomial())
pred <- predict(fit, type = "response")

## with group numbers
perfScores(pred, truth = infert$case, namePos = 1)

## with group names
my.case <- factor(infert$case, labels = c("control", "case"))
pred <- predict(fit)
perfScores(pred, truth = my.case, namePos = "case")

## on the scale of the linear predictors
pred2 <- predict(fit)
pred <- predict(fit)
perfScores(pred2, truth = infert$case, namePos = 1)

## using weights
pred <- predict(fit)
perfScores(pred, truth = infert$case, namePos = 1, wBS = 0.3)
```

predValues

*Compute PPV and NPV.*

Description

The function computes the positive (PPV) and negative predictive value (NPV) given sensitivity, specificity and prevalence (pre-test probability).

Usage

```
predValues(sens, spec, prev)
```

Arguments

```
sens numeric vector: sensitivities.
spec numeric vector: specificities.
prev numeric vector: prevalence.
```

Details

The function computes the positive (PPV) and negative predictive value (NPV) given sensitivity, specificity and prevalence (pre-test probability).

It's a simple application of the Bayes formula.

One can also specify vectors of length larger than 1 for sensitivity and specificity.

Value

Vector or matrix with PPV and NPV.
Author(s)
Matthias Kohl <Matthias.Kohl@stamats.de>

Examples

```r
## Example: HIV test
## 1. ELISA screening test (4th generation)
predValues(sens = 0.999, spec = 0.998, prev = 0.001)
## 2. Western-Plot confirmation test
predValues(sens = 0.998, spec = 0.999996, prev = 1/3)
```

```r
## Example: connection between sensitivity, specificity and PPV
sens <- seq(0.6, 0.99, by = 0.01)
spec <- seq(0.6, 0.99, by = 0.01)
ppv <- function(sens, spec, pre) predValues(sens, spec, pre)
res <- outer(sens, spec, ppv, pre = 0.1)
image(sens, spec, res, col = terrain.colors(256), main = "PPV for prevalence = 10%",
     xlim = c(0.59, 1), ylim = c(0.59, 1))
contour(sens, spec, res, add = TRUE)
```

---

**risks**

*Compute RR, OR and Other Risk Measures*

Description

The function computes relative risk (RR), odds ration (OR), and several other risk measures; see details.

Usage

```r
risks(p0, p1)
```

Arguments

- `p0`: numeric vector of length 1: incidence of the outcome of interest in the nonexposed group.
- `p1`: numeric vector of length 1: incidence of the outcome of interest in the exposed group.

Details

The function computes relative risk (RR), odds-ratio (OR), relative risk reduction (RRR) resp. relative risk increase (RRI), absolute risk reduction (ARR) resp. absolute risk increase (ARI), number needed to treat (NNT) resp. number needed to harm (NNH).

Value

Vector including several risk measures.
**rrCI**

**Author(s)**
Matthias Kohl <Matthias.Kohl@stamats.de>

**References**

**Examples**
```r
## See worked example in Wikipedia
risks(p0 = 0.4, p1 = 0.1)
risks(p0 = 0.4, p1 = 0.5)
```

---

**rrCI**

*Compute Approximate Confidence Interval for RR.*

**Description**
The function computes an approximate confidence interval for the relative risk (RR).

**Usage**
```r
rrCI(a, b, c, d, conf.level = 0.95)
```

**Arguments**
- **a** integer: events in exposed group.
- **b** integer: non-events in exposed group.
- **c** integer: events in non-exposed group.
- **d** integer: non-events in non-exposed group.
- **conf.level** numeric: confidence level

**Details**
The function computes an approximate confidence interval for the relative risk (RR) based on the normal approximation; see Jewell (2004).

**Value**
A list with class "confint" containing the following components:
- **estimate** the estimated relative risk.
- **conf.int** a confidence interval for the relative risk.
Author(s)

Matthias Kohl <Matthias.Kohl@stamats.de>

References


Examples

```r
rrCI(a = 15, b = 135, c = 100, d = 150)
rrCI(a = 75, b = 75, c = 100, d = 150)
```
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