

Package ‘mlquantify’

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Type Package

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Description Quantification is a prominent machine learning task that has received an increasing amount of attention in the last years. The objective is to predict the class distribution of a data sample. This package is a collection of machine learning algorithms for class distribution estimation. This package include algorithms from different paradigms of quantification. These methods are described in the paper: A. Maletzke, W. Hassan, D. dos Reis, and G. Batista. The importance of the test set size in quantification assessment. In Proceedings of the Twenty-Ninth International Joint Conference on Artificial Intelligence, IJCAI20, pages 2640–2646, 2020. <doi:10.24963/ijcai.2020/366>.

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URL <https://github.com/andregustavom/mlquantify>

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| | |
|-----|------------------------------------|
| ACC | <i>Adjusted Classify and Count</i> |
|-----|------------------------------------|

Description

It quantifies events based on testing scores using the Adjusted Classify and Count (ACC) method. ACC is an extension of CC, applying a correction rate based on the true and false positive rates (tpr and fpr).

Usage

```
ACC(test, TprFpr, thr=0.5)
```

Arguments

| | |
|--------|---|
| test | a numeric vector containing the score estimated for the positive class from each test set instance. |
| TprFpr | a data.frame of true positive (tpr) and false positive (fpr) rates estimated on training set, using the function getTPRandFPRbyThreshold(). |
| thr | threshold value according to the tpr and fpr were learned. Default is 0.5. |

Value

A numeric vector containing the class distribution estimated from the test set.

References

Forman, G. (2006, August). Quantifying trends accurately despite classifier error and class imbalance. In ACM SIGKDD international conference on Knowledge discovery and data mining (pp. 157-166).<doi.org/10.1145/1150402.1150423>.

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 3)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
ts <- aeAegypti[cv$Fold3,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
TprFpr <- getTPRandFPRbyThreshold(scores)
test.scores <- predict(scorer, ts_sample, type = c("prob"))
ACC(test = test.scores[,1], TprFpr = TprFpr)
```

aeAegypti

Males and Females Aedes Aegypti data from Maletzke (2019)

Description

Contains events generated by a laser sensor to capture the flight dynamism of insects. It is a binary dataset compose by events from *Aedes Aegypti* Female and Male.

Usage

```
data(aeAegypti)
```

Format

The data set aeAegypti is a data frame of 1800 observations of 9 variables. Each event is described by the wing beat frequency (wbf), and the frequencies of the first six harmonics obtained when either female or male *Aedes Aegypti* mosquito cross an optical sensor's line-of-sigh. Both male (class = 2) and female (class = 1) of class factor.

Details

The aeAegypti dataset is a subset of widely data collection effort involving more than one million instances from 20 different insect species. The dataset was collected varying the temperature and humidity. An observation is associated with a temperature range that varies from 23°C to 35°C.

Author(s)

Andre Maletzke <andregustavom@gmail.com>

References

Maletzke, A. G. (2019). Binary quantification in non-stationary scenarios. Doctoral Thesis, Instituto de Ciências Matemáticas e de Computação, University of São Paulo, São Carlos. Retrieved 2020-07-21, from www.teses.usp.br. <doi.org/10.11606/T.55.2020.tde-19032020-091709>

Moreira dos Reis, D., Maletzke, A., Silva, D. F., & Batista, G. E. (2018). Classifying and counting with recurrent contexts. In Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining (pp. 1983-1992). <doi.org/10.1145/3219819.3220059>

CC

Classify and Count

Description

It quantifies events based on testing scores, applying the Classify and Count (CC). CC is the simplest quantification method that derives from classification (Forman, 2005).

Usage

```
CC(test, thr=0.5)
```

Arguments

| | |
|------|---|
| test | a numeric vector containing the score estimated for the positive class from each test set instance. |
| thr | a numeric value indicating the decision threshold. A value between 0 and 1 (default = 0.5) |

Value

A numeric vector containing the class distribution estimated from the test set.

References

Forman, G. (2005). Counting positives accurately despite inaccurate classification. In European Conference on Machine Learning. Springer, Berlin, Heidelberg. <doi.org/10.1007/11564096_55>.

Examples

```

library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 2)
tr <- aeAegypti[cv$Fold1,]
ts <- aeAegypti[cv$Fold2,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
test.scores <- predict(scorer, ts_sample, type = c("prob"))
CC(test = test.scores[,1])

```

DyS

*DyS Framework***Description**

DyS is a framework for quantification data based on mixture models method. It quantifies events based on testing scores, applying the DyS framework proposed by Maletzke et al. (2019). It also works with several similarity functions.

Usage

```
DyS(p.score, n.score, test, measure="topsoe", bins=seq(2,20,2), err=1e-5)
```

Arguments

| | |
|---------|--|
| p.score | a numeric vector of positive scores estimated either from a validation set or from a cross-validation method. |
| n.score | a numeric vector of negative scores estimated either from a validation set or from a cross-validation method. |
| test | a numeric vector containing the score estimated for the positive class from each test set instance. |
| measure | measure used to compare the mixture histogram against the histogram obtained from the test set. Several functions can be used (Default: "topsoe", "euclidean", "jensen_difference", "prob_symm", "taneja", "ord"). |
| bins | a numeric vector of number of bins used to construct the histogram for representing the score distribution. (default: seq(2, 20, 2)). |
| err | a numeric value defining the accepted error for the ternary search (default: 1e5). |

Value

A numeric vector containing the class distribution estimated from the test set.

References

Maletzke, A., Reis, D., Cherman, E., & Batista, G. (2019). DyS: a Framework for Mixture Models in Quantification. in Proceedings of the The Thirty-Third AAAI Conference on Artificial Intelligence, ser. AAAI'19, 2019. <doi.org/10.1609/aaai.v33i01.33014552>.

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 3)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
ts <- aeAegypti[cv$Fold3,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
test.scores <- predict(scorer, ts_sample, type = c("prob"))
DyS(p.score = scores[scores[,3]==1,1], n.score = scores[scores[,3]==2,1],
    test = test.scores[,1])
```

EMQ

Expectation-Maximization Quantification

Description

This method is an instance of the well-known algorithm for finding maximum-likelihood estimates of the model's parameters. It quantifies events based on testing scores, applying the Expectation Maximization for Quantification (EMQ) method proposed by Saerens et al. (2002).

Usage

```
EMQ(train, test, it=5, e=1e-4)
```

Arguments

| | |
|--------------------|---|
| <code>train</code> | a data.frame of the labeled set. |
| <code>test</code> | a numeric matrix of scores predicted from each test set instance. First column must be the positive score. |
| <code>it</code> | maximum number of iteration steps (default 5). |
| <code>e</code> | a numeric value for the stop threshold (default 1e-4). If the difference between two consecutive steps is lower or equal than e, the iterative process will be stopped. If e is null then the iteration phase is defined by the it parameter. |

Value

A numeric vector containing the class distribution estimated from the test set.

References

Saerens, M., Latinne, P., & Decaestecker, C. (2002). Adjusting the outputs of a classifier to new a priori probabilities: a simple procedure. *Neural computation*.<doi.org/10.1162/089976602753284446>.

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 2)
tr <- aeAegypti[cv$Fold1,]
ts <- aeAegypti[cv$Fold2,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
test.scores <- predict(scorer, ts_sample, type = c("prob"))
EMQ(train=tr, test=test.scores)
```

getTPRandFPRbyThreshold

Estimates true and false positive rates

Description

This function provides the true and false positive rates (tpr and fpr) for a range of thresholds.

Usage

```
getTPRandFPRbyThreshold(validation_scores, label_pos = 1, thr_range = seq(0,1,0.01))
```

Arguments

| | |
|-------------------|---|
| validation_scores | data.frame scores estimated from the training set. It should be comprised of three columns (1. positive scores; 2. negative scores; 3.class). |
| label_pos | numeric value or factor indicating the positive label. |
| thr_range | a numerical vector of thresholds, ranged between 0 and 1. Default: seq(0.01, 0.99, 0.01). |

Value

data.frame where each row has both (tpr and fpr) rates for each threshold value. This function varies the threshold from 0.01 to 0.99 with increments 0.01.

Author(s)

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Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 2)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
TprFpr <- getTPRandFPRbyThreshold(scores)
```

HDy_LP

HDy with Laplace smoothing

Description

It computes the class distribution using the HDy algorithm proposed by González-Castro et al. (2013) with Laplace smoothing (Maletzke et al. (2019)).

Usage

```
HDy_LP(p.score, n.score, test)
```

Arguments

| | |
|---------|---|
| p.score | a numeric vector of positive scores estimated either from a validation set or from a cross-validation method. |
| n.score | a numeric vector of negative scores estimated either from a validation set or from a cross-validation method. |
| test | a numeric vector containing the score estimated for the positive class from each test set instance. |

Value

A numeric vector containing the class distribution estimated from the test set.

Author(s)

Andre Maletzke <andregustavom@gmail.com>

References

González-Castro, V., Alaíz-Rodríguez, R., & Alegre, E. (2013). Class distribution estimation based on the Hellinger distance. *Information Sciences*.<doi.org/10.1016/j.ins.2012.05.028>

Maletzke, A., Reis, D., Cherman, E., & Batista, G. (2019). DyS: a Framework for Mixture Models in Quantification. in *Proceedings of the The Thirty-Third AAAI Conference on Artificial Intelligence*, ser. AAAI'19, 2019. <doi.org/10.1609/aaai.v33i01.33014552>.

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 3)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
ts <- aeAegypti[cv$Fold3,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
test.scores <- predict(scorer, ts_sample, type = c("prob"))
HDy_LP(p.score = scores[scores[,3]==1,1], n.score=scores[scores[,3]==2,1],
       test=test.scores[,1])
```

KUIPER

Quantification method based on Kuiper's test

Description

It quantifies events based on testing scores, applying an adaptation of the Kuiper's test for quantification problems.

Usage

```
KUIPER(p.score, n.score, test)
```

Arguments

| | |
|---------|---|
| p.score | a numeric vector of positive scores estimated either from a validation set or from a cross-validation method. |
| n.score | a numeric vector of negative scores estimated either from a validation set or from a cross-validation method. |
| test | a numeric vector containing the score estimated for the positive class from each test set instance. |

Value

A numeric vector containing the class distribution estimated from the test set.

Author(s)

Denis dos Reis <denismr@gmail.com>

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 3)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
ts <- aeAegypti[cv$Fold3,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
test.scores <- predict(scorer, ts_sample, type = c("prob"))
KUIPER(p.score = scores[scores[,3]==1,1], n.score = scores[scores[,3]==2,1],
       test = test.scores[,1])
```

MAX

Threshold selection method

Description

It quantifies events based on testing scores, applying MAX method, according to Forman (2006). Same as T50, but it sets the threshold where tpr-fpr is maximized.

Usage

```
MAX(test, TprFpr)
```

Arguments

| | |
|--------|---|
| test | a numeric vector containing the score estimated for the positive class from each test set instance. |
| TprFpr | a data.frame of true positive (tpr) and false positive (fpr) rates estimated on training set, using the function <code>getTPRandFPRbyThreshold()</code> . |

Value

A numeric vector containing the class distribution estimated from the test set.

References

Forman, G. (2006, August). Quantifying trends accurately despite classifier error and class imbalance. In Proceedings of the 12th ACM SIGKDD international conference on Knowledge discovery and data mining (pp. 157-166).<doi.org/10.1145/1150402.1150423>.

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 3)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
ts <- aeAegypti[cv$Fold3,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
TprFpr <- getTPRandFPRbyThreshold(scores)
test.scores <- predict(scorer, ts_sample, type = c("prob"))
MAX(test=test.scores[,1], TprFpr=TprFpr)
```

MKS

Mixable Kolmogorov Smirnov

Description

It quantifies events based on testing scores, applying the Mixable Kolmogorov Smirnov (MKS) method proposed by Maletzke et al. (2019).

Usage

```
MKS(p.score, n.score, test)
```

Arguments

| | |
|---------|---|
| p.score | a numeric vector of positive scores estimated either from a validation set or from a cross-validation method. |
| n.score | a numeric vector of negative scores estimated either from a validation set or from a cross-validation method. |
| test | a numeric vector containing the score estimated for the positive class from each test set instance. |

Value

A numeric vector containing the class distribution estimated from the test set.

References

Maletzke, A., Reis, D., Cherman, E., & Batista, G. (2019). DyS: a Framework for Mixture Models in Quantification. in Proceedings of the The Thirty-Third AAAI Conference on Artificial Intelligence, ser. AAAI'19, 2019.<doi.org/10.1609/aaai.v33i01.33014552>

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 3)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
ts <- aeAegypti[cv$Fold3,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
test.scores <- predict(scorer, ts_sample, type = c("prob"))
MKS(p.score = scores[scores[,3]==1,1], n.score = scores[scores[,3]==2,1],
    test = test.scores)
```

MS

Median Sweep

Description

It quantifies events based on testing scores, applying Median Sweep (MS) method, according to Forman (2006).

Usage

```
MS(test, TprFpr)
```

Arguments

| | |
|--------|---|
| test | a numeric vector containing the score estimated for the positive class from each test set instance. |
| TprFpr | a data.frame of true positive (tpr) and false positive (fpr) rates estimated on training set, using the function <code>getTPRandFPRbyThreshold()</code> . |

Value

A numeric vector containing the class distribution estimated from the test set.

References

Forman, G. (2006, August). Quantifying trends accurately despite classifier error and class imbalance. In Proceedings of the 12th ACM SIGKDD international conference on Knowledge discovery and data mining (pp. 157-166).<doi.org/10.1145/1150402.1150423>.

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 3)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
ts <- aeAegypti[cv$Fold3,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
TprFpr <- getTPRandFPRbyThreshold(scores)
test.scores <- predict(scorer, ts_sample, type = c("prob"))
MS(test = test.scores[,1], TprFpr = TprFpr)
```

MS2

Threshold selection method. Median Sweep

Description

It quantifies events using a modified version of the MS method that considers only thresholds where the denominator (tpr-fpr) is greater than 0.25.

Usage

```
MS2(test, TprFpr)
```

Arguments

| | |
|--------|---|
| test | a numeric vector containing the score estimated for the positive class from each test set instance. |
| TprFpr | a data.frame of true positive (tpr) and false positive (fpr) rates estimated on training set, using the function <code>getTPRandFPRbyThreshold()</code> . |

Value

A numeric vector containing the class distribution estimated from the test set.

References

Forman, G. (2006, August). Quantifying trends accurately despite classifier error and class imbalance. In Proceedings of the 12th ACM SIGKDD international conference on Knowledge discovery and data mining (pp. 157-166).<doi.org/10.1145/1150402.1150423>.

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 3)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
ts <- aeAegypti[cv$Fold3,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
TprFpr <- getTPRandFPRbyThreshold(scores)
test.scores <- predict(scorer, ts_sample, type = c("prob"))
MS2(test = test.scores[,1], TprFpr = TprFpr)
```

PACC

Probabilistic Adjusted Classify and Count

Description

It quantifies events based on testing scores, applying the Probabilistic Adjusted Classify and Count (PACC) method. This method is also called Scaled Probability Average (SPA).

Usage

```
PACC(test, TprFpr, thr=0.5)
```

Arguments

| | |
|--------|--|
| test | a numeric vector containing the score estimated for the positive class from each test set instance. (NOTE: It requires calibrated scores. See calibrate from CORElearn). |
| TprFpr | a data.frame of true positive (tpr) and false positive (fpr) rates estimated on training set, using the function <code>getTPRandFPRbyThreshold()</code> . |
| thr | threshold value according to the tpr and fpr were learned. Default is 0.5. |

Value

A numeric vector containing the class distribution estimated from the test set.

References

Bella, A., Ferri, C., Hernández-Orallo, J., & Ramírez-Quintana, M. J. (2010). Quantification via probability estimators. In IEEE International Conference on Data Mining (pp. 737–742). Sidney.<doi.org/10.1109/ICDM.2010.75>.

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 3)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
ts <- aeAegypti[cv$Fold3,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
TprFpr <- getTPRandFPRbyThreshold(scores)
test.scores <- predict(scorer, ts_sample, type = c("prob"))[,1]

# -- PACC requires calibrated scores. Be aware of doing this before using PACC --
# -- You can make it using calibrate function from the CORElearn package --
# if(requireNamespace("CORElearn")){
#   cal_tr <- CORElearn::calibrate(as.factor(scores[,3]), scores[,1], class1=1,
#   method="isoReg",assumeProbabilities=TRUE)
#   test.scores <- CORElearn::applyCalibration(test.scores, cal_tr)
#}
PACC(test = test.scores, TprFpr = TprFpr)
```

PCC

Probabilistic Classify and Count

Description

It quantifies events based on testing scores, applying the Probabilistic Classify and Count (PCC) method.

Usage

```
PCC(test)
```

Arguments

test a numeric vector containing the score estimated for the positive class from each test set instance. (NOTE: It requires calibrated scores. See [calibrate](#) from **CORElearn**).

Value

A numeric vector containing the class distribution estimated from the test set.

References

Bella, A., Ferri, C., Hernández-Orallo, J., & Ramírez-Quintana, M. J. (2010). Quantification via probability estimators. In IEEE International Conference on Data Mining (pp. 737–742). Sidney.<doi.org/10.1109/ICDM.2010.75>.

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 3)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
ts <- aeAegypti[cv$Fold3,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
test.scores <- predict(scorer, ts_sample, type = c("prob"))[,1]

# -- PCC requires calibrated scores. Be aware of doing this before using PCC --
# -- You can make it using calibrate function from the CORElearn package --
# if(requireNamespace("CORElearn")){
#   cal_tr <- CORElearn::calibrate(as.factor(scores[,3]), scores[,1], class1=1,
#   method="isoReg",assumeProbabilities=TRUE)
#   test.scores <- CORElearn::applyCalibration(test.scores, cal_tr)
# }
PCC(test=test.scores)
```

 PWK

Proportion-weighted k-nearest neighbor

Description

It is a nearest-neighbor classifier adapted for working over quantification problems. This method applies a weighting scheme, reducing the weight on neighbors from the majority class.

Usage

```
PWK(train, y, test, alpha=1, n_neighbors=10)
```


Arguments

| | |
|--------------------------|--|
| <code>train</code> | a <code>data.frame</code> containing the training data. |
| <code>y</code> | a vector containing the target values. |
| <code>test</code> | a <code>data.frame</code> containing the test data. |
| <code>alpha</code> | a numeric value defining the proportion-weighted k-nearest neighbor algorithm as proposed by Barranquero et al., (2012). (Default: 1). |
| <code>n_neighbors</code> | a integer value defining the number of neighbors to use by default for nearest neighbor queries (Default: 10). |

Value

A numeric vector containing the class distribution estimated from the test set.

References

Barranquero, J., González, P., Díez, J., & Del Coz, J. J. (2013). On the study of nearest neighbor algorithms for prevalence estimation in binary problems. *Pattern Recognition*, 46(2), 472-482.<doi.org/10.1016/j.patcog.2012.07.022>

Examples

```
library(caret)
library(FNN)
cv <- createFolds(aeAegypti$class, 2)
tr <- aeAegypti[cv$Fold1,]
ts <- aeAegypti[cv$Fold2,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
PWK(train=tr[,-which(names(tr)=="class")], y=tr["class"], test= ts[,-which(names(ts)=="class")])
```

SMM

Sample Mean Matching

Description

SMM is a member of the DyS framework that uses simple means scores to represent the score distribution for positive, negative, and unlabelled scores. Therefore, the class distribution is given by a closed-form equation.

Usage

```
SMM(p.score, n.score, test)
```

Arguments

| | |
|---------|---|
| p.score | a numeric vector of positive scores estimated either from a validation set or from a cross-validation method. |
| n.score | a numeric vector of negative scores estimated either from a validation set or from a cross-validation method. |
| test | a numeric vector containing the score estimated for the positive class from each test set instance. |

Value

A numeric vector containing the class distribution estimated from the test set.

References

Hassan, W., Maletzke, A., Batista, G. (2020). Accurately Quantifying a Billion Instances per Second. In IEEE International Conference on Data Science and Advanced Analytics (DSAA).

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 3)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
ts <- aeAegypti[cv$Fold3,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
test.scores <- predict(scorer, ts_sample, type = c("prob"))
SMM(p.score = scores[scores[,3]==1,1], n.score = scores[scores[,3]==2,1],
    test = test.scores[,1])
```

SORD

Sample ORD Dissimilarity

Description

It quantifies events based on testing scores applying the framework DyS with the Sample ORD Dissimilarity (SORD) proposed by Maletzke et al. (2019).

Usage

```
SORD(p.score, n.score, test)
```

Arguments

| | |
|---------|---|
| p.score | a numeric vector of positive scores estimated either from a validation set or from a cross-validation method. |
| n.score | a numeric vector of negative scores estimated either from a validation set or from a cross-validation method. |
| test | a numeric vector containing the score estimated for the positive class from each test set instance. |

Value

A numeric vector containing the class distribution estimated from the test set.

References

Maletzke, A., Reis, D., Cherman, E., & Batista, G. (2019). DyS: a Framework for Mixture Models in Quantification. in Proceedings of the The Thirty-Third AAAI Conference on Artificial Intelligence, ser. AAAI'19, 2019.<doi.org/10.1609/aaai.v33i01.33014552>.

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 3)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
ts <- aeAegypti[cv$Fold3,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
test.scores <- predict(scorer, ts_sample, type = c("prob"))
SORD(p.score = scores[scores[,3]==1,1], n.score = scores[scores[,3]==2,1],
test = test.scores[,1])
```

Description

It quantifies events based on testing scores, applying T50 method proposed by Forman (2006). It sets the decision threshold of Binary Classifier where tpr = 50%.

Usage

```
T50(test, TprFpr)
```

Arguments

| | |
|---------------------|---|
| <code>test</code> | a numeric vector containing the score estimated for the positive class from each test set instance. |
| <code>TprFpr</code> | a data.frame of true positive (tpr) and false positive (fpr) rates estimated on training set, using the function <code>getTPRandFPRbyThreshold()</code> . |

Value

A numeric vector containing the class distribution estimated from the test set.

References

Forman, G. (2006, August). Quantifying trends accurately despite classifier error and class imbalance. In Proceedings of the 12th ACM SIGKDD international conference on Knowledge discovery and data mining (pp. 157-166).<doi.org/10.1145/1150402.1150423>.

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 3)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
ts <- aeAegypti[cv$Fold3,]
# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
TprFpr <- getTPRandFPRbyThreshold(scores)
test.scores <- predict(scorer, ts_sample, type = c("prob"))
T50(test=test.scores[,1], TprFpr=TprFpr)
```

X

Threshold selection method

Description

It quantifies events based on testing scores, applying the X method (Forman, 2006). Same as T50, but set the threshold where $(1 - \text{tpr}) = \text{fpr}$.

Usage

```
X(test, TprFpr)
```

Arguments

| | |
|---------------------|---|
| <code>test</code> | a numeric vector containing the score estimated for the positive class from each test set instance. |
| <code>TprFpr</code> | a data.frame of true positive (tpr) and false positive (fpr) rates estimated on training set, using the function <code>getTPRandFPRbyThreshold()</code> . |

Value

A numeric vector containing the class distribution estimated from the test set.

References

Forman, G. (2006, August). Quantifying trends accurately despite classifier error and class imbalance. In Proceedings of the 12th ACM SIGKDD international conference on Knowledge discovery and data mining (pp. 157-166).<doi.org/10.1145/1150402.1150423>.

Examples

```
library(randomForest)
library(caret)
cv <- createFolds(aeAegypti$class, 3)
tr <- aeAegypti[cv$Fold1,]
validation <- aeAegypti[cv$Fold2,]
ts <- aeAegypti[cv$Fold3,]

# -- Getting a sample from ts with 80 positive and 20 negative instances --
ts_sample <- rbind(ts[sample(which(ts$class==1),80),],
                  ts[sample(which(ts$class==2),20),])
scorer <- randomForest(class~., data=tr, ntree=500)
scores <- cbind(predict(scorer, validation, type = c("prob")), validation$class)
TprFpr <- getTPRandFPRbyThreshold(scores)
test.scores <- predict(scorer, ts_sample, type = c("prob"))
X(test=test.scores[,1], TprFpr=TprFpr)
```

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