Package 'switchBox'

October 9, 2015

Version 1.2.0

Date 2014-03-20

Title Utilities to train and validate classifiers based on pair switching using the K-Top-Scoring-Pair (KTSP) algorithm.

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Depends R (>= 2.13.1)

Description The package offer different classifiers based on comparisons of pair of features (TSP), using various decision rules (e.g., majority wins principle).

biocViews Software, StatisticalMethod, Classification

License GPL-2

NeedsCompilation yes

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switchBox-package

Description

The switchBox package allows to train and apply a K-Top-Scoring-Pair (KTSP) classifier with learning mechanism proposed in Afsari et al (AOAS, 2014) and as used by Marchionni et al (BMC Genomics, 2013). KTSP is an extension of the TSP classifier described by Geman and colleagues (Bioinformatics, 2005). The TSP algorithm is a simple binary classifier based on the reversal ordering across phenotypes of two measurements (e.g. gene expression reversals from normal to cancer.

switchBox package features

The switchBox package contains several utilities enabling to:

A) Filter the features to be used to develop the classifier (*i.e.*, differentially expressed genes);

B) Compute the scores for all available feature pairs to identify the top performing TSP;

C) Compute the scores for selected feature pairs to identify the top performing TSP;

D) Identify the number of \$K\$ TSP to be used in the final classifier using the analysis of variance;

E) Compute individual TSP votes for one class or the other and combine the votes based on user defined methods;

F) Classify new samples based on the top KTSP based on various methods.

Author(s)

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References

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Marchionni et al., "A simple and reproducible breast cancer prognostic test.", *BMC Genomics*, 2013, **14**(1):336-342 http://www.ncbi.nlm.nih.gov/pubmed/23682826

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Xu et al., "Robust prostate cancer marker genes emerge from direct integration of inter-study microarray data" *Bioinformatics* (2005) **21**(20), 3905-3911. http://www.ncbi.nlm.nih.gov/pubmed/16131522

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KTSP.Classifiy

Description

KTSP.Classify classifies new test samples using KTSP coming out of the function KTSP.Train. This function was used in Marchionni et al, 2013, BMC Genomics, and it is maintained only for backward compatibility. It has been replaced by SWAP.KTSP.Classify.

Usage

KTSP.Classify(data, classifier, combineFunc)

Arguments

data	the test data: a matrix in which the rows represent the genes and the columns the samples.
classifier	The output of KTSP. Train, a KTSP classifier.
combineFunc	A user defined function to combine the predictions of the individual K TSPs. If missing the consensus classification among the majority of the TSPs will be used.

Author(s)

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References

See switchBox for the references.

See Also

KTSP.Train, SWAP.KTSP.Classify,

Examples

```
table(trainingGroupNum)
```

```
*****
### Train a classifier using default filtering function based on the Wilcoxon test
classifier <- KTSP.Train(matTraining, trainingGroupNum, n=8)</pre>
### Show the classifier
classifier
****
### Testing on new data
### Load the example data for the TEST set
data(testingData)
### Turn into a numeric vector with values equal to 0 and 1
testingGroupNum <- as.numeric(testingGroup) - 1</pre>
### Show group variable for the TEST set
table(testingGroupNum)
### Apply the classifier to one sample of the TEST set using
### sum of votes grearter than 2
testPrediction <- KTSP.Classify(matTesting, classifier,</pre>
    combineFunc = function(x) sum(x) < 2.5
### Show prediction
table(testPrediction, testingGroupNum)
```

KTSP.Train

Funtion for training the K-TSP classifier.

Description

KTSP. Train trains a K-TSP classifier for the specific phenotype of interest. The classifiers resulting from using this function can be passed to KTSP.Classify for samples classification. This function was used in Marchionni et al, 2013, BMC Genomics, and it is maintained only for backward compatibility. It has been replaced by SWAP.KTSP.Train.

Usage

```
KTSP.Train(data, situation, n)
```

Arguments

data	the matrix of the values (usually gene expression) to be used to train the classi- fier. The columns represents samples and the rows represents the genes.
situation	an integer vector containing the training labels. Its elements should be one or zero.

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KTSP.Train

n	The number of disjoint TSP used for classification. If before n pairs, the score
	drops to zero, the TSP with zero score are ignored.

Value

The KTSP classifier, a list containing the following elements:

TSPs	a matrix containing TSPs indexes.
score	a vector containing TSPs scores.
geneNames	a matrix containing TSPs feature names.

It should be passed to KTSP.Classify for classification of test samples.

Author(s)

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References

See switchBox for the references.

See Also

KTSP.Classify,SWAP.KTSP.Train,

Examples

Turn into a numeric vector with values equal to 0 and 1
trainingGroupNum <- as.numeric(trainingGroup) - 1</pre>

Show group variable for the TRAINING set table(trainingGroupNum)

Show the classifier
classifier

```
matTesting
```

Description

A numerical matrix containing gene expression matrix for 70 genes and 307 breast cancer patients (test set data) from the Buyse et al cohort (see the mammaPrintData package).

Usage

data(testingData)

Format

The matTesting matrix contains normalized expression values for the 70 gene signature (rows) across 307 samples (columns). Group information (emph"bad" versus "good" prognosis) is shown in colnames(matTesting).

Details

This dataset corresponds to the breast cancer patients' cohort published by Buyse and colleagues in JNCI (2006). The gene expression matrix was obtained from the mammaPrintData package as described by Marchionni and colleagues in BMC Genomics (2013).

Author(s)

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References

See switchBox for the references.

See Also

matTraining

Examples

Load gene expression data for the test set data(testingData) ### Show the class of the ``matTesting'' object class(matTesting) ### Show the dimentions of the ``matTesting'' matrix dim(matTesting)

Show the first 10 sample names of the ``matTest'' matrix

matTraining

```
head(colnames(matTesting), n=10)
testingGroup[1:10]
```

matTraining

Gene expression matrix for training set data

Description

A numerical matrix containing gene expression matrix for 70 genes and 78 breast cancer patients (training set data) from the Glas et al cohort (see the mammaPrintData package).

Usage

data(trainingData)

Format

The matTraining matrix contains normalized expression values for the 70 gene signature (rows) across 78 samples (columns). Group information (emph"bad" versus "good" prognosis) is shown in colnames(matTraining).

Details

This dataset corresponds to the breast cancer patients' cohort published by Glas and colleagues in BMC Genomics (2006). The gene expression matrix was obtained from the mammaPrintData package as described by Marchionni and colleagues in BMC Genomics (2013).

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References

See switchBox for the references.

See Also

matTesting

Examples

Load gene expression data for the training set data(trainingData)

Show the class of the ``matTraining'' object
class(matTraining)

```
### Show the dimentions of the ``matTraining'' matrix
dim(matTraining)
### Show the first 10 sample names of the ``matTraining'' matrix
head(colnames(matTraining), n=10)
```

SWAP.CalculateSignedScore

Function to calculate the pair-wise scores.

Description

SWAP.CalculateSignedScore calculates the pair-wise scores between features pairs. The user may pass a filtering function to reduce the number of starting features, or provide a restricted set of pairs to limit the reported scores to this list.

Usage

```
SWAP.CalculateSignedScore(inputMat, phenoGroup,
FilterFunc = SWAP.Filter.Wilcoxon, RestrictedPairs, ...)
```

Arguments

inputMat	is a numerical matrix containing the measurements (<i>e.g.</i> , gene expression data) to be used to build the K-TSP classifier. The columns represent samples and the rows represent the features (<i>e.g.</i> , genes). The number of columns must agree with the length of phenoGroup. Note that rownames(inputMat) will be construed as feature names (<i>e.g.</i> , gene symbols) in all subsequent analyses.	
phenoGroup	is a factor containing the training phenotypes with two levels.	
FilterFunc	is a filtering function to reduce the starting number of features to be used to iden- tify the Top Scoring Pairs (TSPs). The default filter is based on the Wilcoxon rank-sum test and alternative filtering functions can be passed too (see SWAP.Filter.Wilcoxon for details). Note the filtering function must return feature names, i.e. a subset of rownames(inputMat).	
RestrictedPairs		
	is a character matrix with two columns containing the feature pairs to be con- sidered for score calculations. Each row should contain a pair of feature names matching the rownames(inputMat). If RestrictedPairs is missing all available feature pairs will be considered.	
	Additional argument passed to the filtering function FilterFunc.	

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Value

The output is a list containing the following items:

labels	the levels (phenotypes) in phenoGroup.
Ρ	<pre>a matrix or a vector containing the probability of comparisons in samples with phenotype equal to label[1]. In case RestrictedPairs is not given, P is a ma- trix and P[i,j] = P(InputMat1[i,] < InputMat2[j,] phenoGroup == \$label[1]). In case RestrictedPairs is given, P[k] = P(InputMat1[RestrictedPairs[k,1],] < InputMat2[RestrictedPairs[k,2],] phenoGroup == \$label[1]).</pre>
Q	a matrix or a vector containing the probability of comparisons in samples with phenotype label[2].
score	a matrix or a vector containing the pair-wise scores. Basically, score = $P - Q + C$. The C term is the tie breaker and proportion to the secondary score to avoid the ties.

Note that the P, Q, and score list elements are matrices when scores are computed for all possible feature pairs, while they are vectors when scores are computed for restricted pairs defined by RestrictedPairs.

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References

See switchBox for the references.

See Also

See SWAP.KTSP.Train, SWAP.Filter.Wilcoxon, and SWAP.KTSP.Statistics.

Examples

Load gene expression data for the training set data(trainingData)

Show group variable for the TRAINING set table(trainingGroup)

Compute the scores using all features (a matrix will be returned)
scores <- SWAP.CalculateSignedScore(matTraining, trainingGroup, FilterFunc=NULL,)</pre>

Show scores
class(scores)
dim(scores\$score)

Get the scores for a couple of features diag(scores\$score[1:3 , 5:7])

```
### Compute the scores using the default filtering function for 20 features
scores <- SWAP.CalculateSignedScore(matTraining, trainingGroup, featureNo=20)
### Show scores
dim(scores$score)
### Creating some random pairs
set.seed(123)
somePairs <- matrix(sample(rownames(matTraining), 25, replace=FALSE), ncol=2)
### Compute the scores for restricted pairs (a vector will be returned)
scores <- SWAP.CalculateSignedScore(matTraining, trainingGroup,
FilterFunc = NULL, RestrictedPairs = somePairs )
### Show scores
class(scores$score)
length(scores$score)</pre>
```

SWAP.Filter.Wilcoxon Statistical feature filtering based on Wilcoxon test on the ranks of expressions.

Description

SWAP.Filter.Wilcoxon filters the features to top differential expressed to be used for KTSP classifier implementation.

Usage

```
SWAP.Filter.Wilcoxon(phenoGroup, inputMat, featureNo = 100, UpDown = TRUE)
```

Arguments

phenoGroup	a factor with levels containing training labels for the phenotype of interest.
inputMat	a numerical matrix containing feature measurements to be used to implement the classifier (<i>e.g.</i> , the set of gene expression values). The columns of this matrix correspond to samples and must correspond to phenoGroup. The rows represent the features and rownames(inputMat) will be used as feature names.
featureNo	an integer specifying the number of different features to be returned.
UpDown	logical value specifying whether an equal proportion of features displaying opposite change across the two phenotypes should be returned (<i>e.g.</i> an equal number of up- and down-regulated genes).

Value

The names of the features that survived the statistical filtering, i.e. differential expressed features.

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References

See switchBox for the references.

See Also

```
SWAP.KTSP.Classify,SWAP.Filter.Wilcoxon,SWAP.CalculateSignedScore
```

Examples

```
### Load gene expression data for the training set
data(trainingData)
```

Return equal numbers of up- and down- regulated features (default)
SWAP.Filter.Wilcoxon(trainingGroup, matTraining, featureNo=10)

Return the top 10 differentially expressed features irrispective to
the direction of change.
By setting the argument 'UpDown' equal to FALSE the number of
up- and down- regulated features can be different
SWAP.Filter.Wilcoxon(trainingGroup, matTraining, featureNo=10, UpDown=FALSE)

SWAP.KTSP.Classifiy Function to classify samples using a KTSP classifier.

Description

SWAP.KTSP.Classify classifies new test samples using KTSP coming out of the function SWAP.KTSP.Train.

Usage

```
SWAP.KTSP.Classify(inputMat, classifier, DecisionFunc)
```

Arguments

inputMat	is a numerical matrix containing the measurements (<i>e.g.</i> , gene expression data) to be used with a K-TSP classifier to classify the samples in a specific class or the other. In this numerical matrix the columns represent the samples and the rows represent the features (<i>e.g.</i> , genes) used by the classification rule. Note that rownames(inputMat) will be used to select the features (<i>e.g.</i> , gene symbols)
	contained in the K-TSP classifier.
classifier	the classifier obtained by invoking SWAP.KTSP.Train.

DecisionFunc is the function used to generate the final classification prediction by combining the comparisons of the TSPs in the classifier. By default each sample is classified according to the class voted by the majority of the TSPs ("majority wins" principle). Different decision rules can be also specified using alternative functions passed DecisionFunc, as described below (see "details").

Details

The SWAP.KTSP.Classify classifies new test samples based on a specific decision rule. By default, each sample is classified based on the the majority voting rule of the comparisons of TSPs in the classifier. Alternative rules can be defined by the user and passed to SWAP.KTSP.Classify using the argument DecisionFunc. A decision function takes as its input a logical vector x corresponding to the individual decision of each TSP (TRUE if the first feature in the pair is larger then the second, FALSE in the opposite case). The output of the DecisionFunction is a single logical value summarizing all votes of the individual TSPs (see examples below).

Value

This function returns the predicted class for each sample in the form of a factor.

Author(s)

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References

See switchBox for the references.

See Also

SWAP.KTSP.Train, SWAP.Filter.Wilcoxon, SWAP.CalculateSignedScore

Examples

Show group variable for the TRAINING set table(trainingGroup)

Show the classifier
classifier

SWAP.KTSP.Statistics

```
### Apply the classifier to the TRAINING set using default decision rule
trainingPrediction <- SWAP.KTSP.Classify(matTraining, classifier)</pre>
```

```
### Resubstitution performance in the TRAINING set
### Define a "positive" test result if needed
table(trainingPrediction, trainingGroup)
```

```
### Use an alternative DecideFunction to classify each patient
### Here for instance at least two TSPs must agree
trainingPrediction <- SWAP.KTSP.Classify(matTraining, classifier,
    DecisionFunc = function(x) sum(x) > 5.5 )
```

Contingency table for the TRAINING set table(trainingPrediction, trainingGroup)

Load the example data for the TEST set data(testingData)

```
### Show group variable for the TEST set
table(testingGroup)
```

Apply the classifier to one sample of the TEST set using default decision rule testPrediction <- SWAP.KTSP.Classify(matTesting[, 1, drop=FALSE], classifier)</pre>

```
### Show prediction
testPrediction
```

Show prediction
head(testPrediction, n=10)

```
### Contingency table for the TEST set
table(testPrediction, testingGroup)
```

SWAP.KTSP.Statistics Function computing TSP votes (comparisons) and combine their votes. The default is the kTSP statistics, sum of the votes.

Description

SWAP.KTSP.Statistics computes the votes in favor of one of the classes or the other for each TSP. This function also computes the final, combined, consensus of all TSP votes based on a specific decision rules. The default is the kTSP statistics, sum of the votes.

Usage

SWAP.KTSP.Statistics(inputMat, classifier, CombineFunc)

Arguments

inputMat	is a numerical matrix containing the measurements (<i>e.g.</i> , gene expression data) to be used to compute the individual TSP votes and their consensus. like the matrix used for training classifier (in SWAP.KTSP.Train function), inputMatrix rows represent the features and the columns represent the samples.
classifier	the classifier obtained by invoking SWAP.KTSP.Train.
CombineFunc	is the function used to combine the votes (i.e., comparisons) of individual TSPs contained in the classifier. By default, the consensus is the count of the votes taking into account the order of the features in each TSP. Using this argument alternative aggregating functions can be also passed to SWAP.KTSP.Statistics as described below (see "details").

Details

For each TSP in the KTSP classifier, SWAP.KTSP.Statistics computes the vote in favor of one of classes or the other. This function also aggregates the individual TSP votes and computes a final consensus of all TSP votes based on specific combination rules. By default, this combination is achieved by counting the comparisons (votes) of TSPs as follows: If the first feature is larger than the second one, the TSP vote is positive, else the TSP vote is negative. Different combination rules can also be specified by defining an alternative combination function and by passing it to SWAP.KTSP.Statistics using the CombineFunc argument. A combination function takes as its input a logical vector x corresponding to the sample TSP comparisons (TRUE if the first feature in the pair is larger then the second, FALSE in the opposite case). The output of the CombineFunction is a single value summarizing the votes of all individual TSPs (see examples below). Note that CombineFunction function must operate on a logical vector as input and the outcome must be real value number.

Value

A list containing the following two components:

statistics a named vector containing the aggregated summary statistics computed by CombineFunc. The names correspond to samples and are derived from colnames(inputMat).
 comparisons a logical matrix containing the individual TSP votes (TRUE if the first pair feature is larger then the second one, FALSE otherwise). The columns of this matrix correspond to TSP comparisons and are named accordingly using feature names derived from rownames(inputMat). The columns of this matrix correspond to the samples and are named accordingly using colnames(inputMat).

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References

See switchBox for the references.

See Also

SWAP.KTSP.Classify, SWAP.Filter.Wilcoxon, SWAP.CalculateSignedScore

Examples

Show group variable for the TRAINING set table(trainingGroup)

Show the TSP in the classifier
classifier\$TSPs

```
### Show components
names(ktspStatDefault)
```

```
### Show some of the votes
head(ktspStatDefault$comparisons[ , 1:2])
```

```
### Show default statistics
head(ktspStatDefault$statistics)
### Show statistics obtained using the sum
head(ktspStatSum$statistics)
### Show statistics obtained using the hard threshold
head(ktspStatThreshold)
### Make a heatmap showing the individual TSPs votes
colorForRows <- as.character(1+as.numeric(trainingGroup))
heatmap(1*ktspStatDefault$comparisons, scale="none",
margins = c(10, 5), cexCol=0.5, cexRow=0.5,
labRow=trainingGroup, RowSideColors=colorForRows)
```

SWAP.KTSP.Train Function for training the K-TSP classifier.

Description

SWAP.KTSP.Train trains a binary K-TSP classifier. The classifiers resulting from using this function can be passed to SWAP.KTSP.Classify for samples classification.

Usage

```
SWAP.KTSP.Train(inputMat, phenoGroup, krange = c(3, 5, 7:10),
FilterFunc = SWAP.Filter.Wilcoxon, RestrictedPairs, ...)
```

Arguments

inputMat	is a numerical matrix containing the measurements (<i>e.g.</i> , gene expression data) to be used to build the K-TSP classifier. The columns represent samples and the rows represent the features (<i>e.g.</i> , genes). The number of columns must agree with the length of phenoGroup. Note that rownames(inputMat) will be used as the feature names (<i>e.g.</i> , gene symbols) in all subsequent analyses.
phenoGroup	is a factor with two levels containing the phenotype information used to train the K-TSP classifier. In order to identify the best TSP to be included in the classifier, the features contained in inputMat will be compared between the two groups defined by this factor. Levels from phenoGroup will be also used to reorder the features in each TSP such as the first feature is larger than the second one in the group corresponding to first level, and <i>vice-versa</i> .
krange	an integer (or a vector of integers) defining the candidate number of Top Scoring Pairs (TSPs) from which the algorithm chooses to build the final classifier. The algorithm uses the mechanism in Afsari et al (AOAS, 2014) to select the number of pairs and pair of features.

FilterFunc	is a filtering function to reduce the starting number of features to be used to iden- tify the Top Scoring Pairs (TSP). The default filter is differential expression test	
	based on the Wilcoxon rank-sum test and alternative filtering functions can be	
	passed too (see SWAP.Filter.Wilcoxon for details). The output of the function	
	<pre>must be subset of rownames(inputMat)</pre>	
RestrictedPairs		
	is a character matrix with two columns containing the feature pairs to be con- sidered for score calculations. Each row should contain a pair of feature names matching the rownames of inputMat. If RestrictedPairs is missing all available feature pairs will be considered.	
	Additional argument passed to the filtering function FilterFunc.	

Value

The KTSP classifier, in the form of a list, which contains the following components:

name	The classifier name.
TSPs	A k by 2 matrix, containing the feature names for each TSP. These names corre- spond to the rownames(inputData). In this matrix each row corresponds to a specific TSP. For each TSP (<i>i.e.</i> row in the TSPs matrix) the order of the features is such that the first one is on average smaller than the second one in the pheno- typic group defined by the first levels of the phenoGroup factor and <i>vice-versa</i> . The algorithm uses the mechanism in Afsari et al (2014) to select the number of pairs and pair of features.
\$score	scores TSP for the top k TSPs.
\$label	The class labels. These labels correspond to the phenoGroup factor lelves and will be used lable any new sample classified by the SWAP.KTSP.Classify function.

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References

See switchBox for the references.

See Also

SWAP.KTSP.Classify,SWAP.Filter.Wilcoxon,SWAP.CalculateSignedScore

Examples

SWAP.KTSP.Train

Show group variable for the TRAINING set table(trainingGroup)

Train a classifier using default filtering function based on the Wilcoxon test classifier <- SWAP.KTSP.Train(matTraining, trainingGroup, krange=c(3, 5, 8:15))</pre>

Show the classifier
classifier

Show the classifier
classifier

To use all features "FilterFunc" must be set to NULL classifier <- SWAP.KTSP.Train(matTraining, trainingGroup, FilterFunc=NULL)</pre>

Show the classifier
classifier

```
### Train a classifier using and alternative filtering function.
### For instance we can use the a "t.test" to selec the features
### with an absolute t-statistics larger than a specified quantile
topRttest <- function(situation, data, quant = 0.75) {
  out <- apply(data, 1, function(x, ...) t.test(x ~ situation)$statistic )
  names(out[ abs(out) > quantile(abs(out), quant) ])
}
```

Show the top features selected topRttest(trainingGroup, matTraining, quant=0.95)

Show the classifier
classifier

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testingGroup

Testing set phenotypes

Description

A factor with two levels describing the phenotypes for the testing data (Buyse et al cohort, (see the mammaPrintData package).

Usage

```
data(testingData)
```

Format

The matTesting factor contains phenotypic information for the 307 samples of the testing dataset.

Details

This phenotype factor corresponds to the breast cancer patients' cohort published by Buyse and colleagues in JNCI (2006). The gene expression matrix was obtained from the mammaPrintData package as described by Marchionni and colleagues in BMC Genomics (2013).

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References

See switchBox for the references.

See Also

trainingGroup

Examples

```
### Load gene expression data for the test set
data(testingData)
### Show the class of the ``testingGroup'' object
class(testingGroup)
### Show group variable
table(testingGroup)
```

trainingGroup Training set phenotypes

Description

A factor with two levels describing the phenotypes for the training data (Glas et al cohort, see the mammaPrintData package).

Usage

```
data(trainingData)
```

Format

The trainingGroup factor contains phenotypic information for the 78 samples of the training dataset.

Details

This phenotype factor corresponds to the breast cancer patients' cohort published by Glas and colleagues in BMC Genomics (2006). The information was obtained from the mammaPrintData package as described by Marchionni and colleagues in BMC Genomics (2013).

Author(s)

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References

See switchBox for the references.

See Also

testingGroup

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trainingGroup

Examples

Load gene expression data for the training set
data(trainingData)

Show the class of the ``trainingGroup'' object
class(trainingGroup)

Show group variable
table(trainingGroup)

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