Package 'CMA'

October 21, 2025

Type Package

Title Synthesis of microarray-based classification

Version 1.67.0

Date 2009-09-14

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Depends R (>= 2.10), methods, stats, Biobase

Suggests MASS, class, nnet, glmnet, e1071, randomForest, plsgenomics,
gbm, mgcv, corpcor, limma, st, mvtnorm

Description This package provides a comprehensive collection of various microarray-
based classification algorithms
both from Machine Learning and Statistics.
Variable Selection, Hyperparameter tuning, Evaluation and Comparison can be performed
combined or stepwise in a user-friendly environment.

Collate classes.r GenerateLearningsets.r GeneSelection.r tune.r
classification.r evaluation.r join.r compare.r Planarplot.r
compBoostCMA.r dldaCMA.r ElasticNetCMA.r fdaCMA.r flexdaCMA.r
gbmCMA.r knnCMA.r LassoCMA.r ldaCMA.r nnetCMA.r pknnCMA.r
plrCMA.r pls_ldaCMA.r pls_lrCMA.r pls_rfCMA.r pnnCMA.r qdaCMA.r
rfCMA.r scdaCMA.r weighted_mcr.r wmc.r shrinkldaCMA.r svmCMA.r
filter.r internals.r

License GPL (>= 2)

biocViews Classification, DecisionTree

git_url https://git.bioconductor.org/packages/CMA

git_branch devel

git_last_commit fb7d8ea

git_last_commit_date 2025-04-15

Repository Bioconductor 3.22

Date/Publication 2025-10-21

Contents

`CMA-package` *Synthesis of microarray-based classification*

Description

The aim of the package is to provide a user-friendly environment for the evaluation of classification methods using gene expression data. A strong focus is on combined variable selection, hyperparameter tuning, evaluation, visualization and comparison of (up to now) 21 classification methods from three main fields: Discriminant Analysis, Neural Networks and Machine Learning. Although the package has been created with the intention to be used for Microarray data, it can as well be used in various `(p > n)`-scenarios.

Details

Package:	CMA
Type:	Package
Version:	1.3.3
Date:	2009-9-14
License:	GPL (version 2 or later)

Most Important Steps for the workflow are:

1. Generate evaluation datasets using `GenerateLearningsets`
2. (Optionally): Perform variable selection using `GeneSelection`
3. (Optionally): Peform hyperparameter tuning using `tune`
4. Perform `classification` using 1.-3.
5. Repeat 2.-4. based on 1. for several methods: `compBoostCMA`, `dldaCMA`, `ElasticNetCMA`, `fdaCMA`, `flexdaCMA`, `gbmCMA`, `knnCMA`, `ldaCMA`, `LassoCMA`, `nnetCMA`, `pknnCMA`, `plrCMA`, `pls_ldaCMA`, `pls_lrCMA`, `pls_rfCMA`, `pnnCMA`, `qdaCMA`, `rfCMA`, `scdaCMA`, `shrinkldaCMA`, `svmCMA`
6. Evaluate the results from 5. using `evaluation` and make a comparison by calling `compare`

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References

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

`Barplot` *Barplot of variable importance*

Description

This method can be seen as a visual pendant to `toplist`. The plot visualizes variable importance by a barplot. The height of the barplots correspond to variable importance. What variable importance exactly means depends on the method chosen when calling `GeneSelection`, s. `genesel`.

Arguments

`x`	An object of class `genesel`
`top`	Number of top genes whose variable importance should be displayed. Defaults to 10.
`iter`	Iteration number (`learningset`) for which variable importance should be displayed.
`...`	Further graphical options passed to `barplot`.

Value

No return.

Note

Note the following

- If `scheme = "multiclass"`, only one plot will be made. Otherwise, one plot will be made for each binary scenario (depending on whether `"scheme"` is `"one-vs-all"` or `"pairwise"`).
- Variable importance do not make sense for variable selection (ranking) methods that are essentially discrete, such as the Wilcoxon-Rank sum statistic or the Kruskal-Wallis statistic.
- For the methods `"lasso"`, `"elasticnet"`, `"boosting"` the number of nonzero coefficients can be very small, resulting in bars of height zero if `top` has been chosen too large.

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References

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

See Also

`genesel`, `GeneSelection`, `toplist`

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best *Show best hyperparameter settings*

Description

In this package hyperparameter tuning is performed by an inner cross-validation step for each `learningset`. A grid of values is tried and evaluated in terms of the misclassification rate, the results are saved in an object of class `tuningresult`. This method displays (separately for each `learningset`) the hyperparameter/ hyperparameter combination that showed the best results. Note that this must not be unique; in this case, only one combination is displayed.

Usage

```
best(object, ...)
```

Arguments

`object`	An object of class `tuningresult`.
`...`	Currently unused argument.

Value

A list with elements equal to the number of different learningsets. Each element contains the best hyperparameter combination and the corresponding misclassification rate.

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See Also

tune

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boxplot *Make a boxplot of the classifier evaluation*

Description

This method displays the slot scores of performance scores of an object of class evaloutput.

Arguments

x	An object of class evaloutput.
...	Further graphical parameters passed to the classical boxplot function.

Value

The only return is a boxplot.

Author(s)

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References

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

See Also

evaluation

`classification` *General method for classification with various methods*

Description

Most general function in the package, providing an interface to perform variable selection, hyperparameter tuning and classification in one step. Alternatively, the first two steps can be performed separately and can then be plugged into this function.
For S4 method information, s. `classification-methods`.

Usage

```
classification(X, y, f, learningsets, genesel, genesellist = list(), nbgene, classifier, tuneres, tu
```

Arguments

`X`	Gene expression data. Can be one of the following: • A `matrix`. Rows correspond to observations, columns to variables. • A `data.frame`, when `f` is *not* missing (s. below). • An object of class `ExpressionSet`.
`y`	Class labels. Can be one of the following: • A `numeric` vector. • A `factor`. • A `character` if `X` is an `ExpressionSet` that specifies the phenotype variable. • `missing`, if `X` is a `data.frame` and a proper formula `f` is provided. **WARNING**: The class labels will be re-coded to range from `0` to `K-1`, where `K` is the total number of different classes in the learning set.
`f`	A two-sided formula, if `X` is a `data.frame`. The left part correspond to class labels, the right to variables.
`learningsets`	An object of class `learningsets`. May be missing, then the complete datasets is used as learning set.
`genesel`	Optional (but usually recommended) object of class `genesel` containing variable importance information for the argument `learningsets`
`genesellist`	In the case that the argument `genesel` is missing, this is an argument list passed to `GeneSelection`. If both `genesel` and `genesellist` are missing, no variable selection is performed.
`nbgene`	Number of best genes to be kept for classification, based on either `genesel` or the call to `GeneSelection` using `genesellist`. In the case that both are missing, this argument is not necessary. **note**: • If the gene selection method has been one of `"lasso"`, `"elasticnet"`, `"boosting"`, `nbgene` will be reset to `min(s, nbgene)` where `s` is the number of nonzero coefficients. • if the gene selection scheme has been `"one-vs-all"`, `"pairwise"` for the multiclass case, there exist several rankings. The top `nbgene` will be kept of *each* of them, so the number of effective used genes will sometimes be much larger.

classifier	Name of function ending with CMA indicating the classifier to be used.
tuneres	Analogous to the argument genesel - object of class tuningresult containing information about the best hyperparameter choice for the argument learningsets.
tuninglist	Analogous to the argument genesellist. In the case that the argument tuneres is missing, this in argument list passed to tune. If both tuneres and tuninglist are missing, no variable selection is performed. **warning**: Note that if a user-defined hyperparameter grid is passed, this will result in a list within a list: tuninglist = list(grids=list(argname = c()), s. example. **warning**: Contrary to tune, if tuninglist is an empty list (default), *no* hyperparameter tuning will be performed at all. To use pre-defined hyperparameter grids, the argument is tuninglist = list(grids = list()).
trace	Should progress be traced ? Default is TRUE.
models	a logical value indicating whether the model object shall be returned
...	Further arguments passed to the function classifier.

Details

For details about hyperparameter tuning, consult tune.

Value

A list of objects of class cloutput and clvarseloutput, respectively; its length equals the number of different learningsets. The single elements of the list can conveniently be combined using the join function. The results can be analyzed and evaluated by various measures using the method evaluation.

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References

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

See Also

GeneSelection, tune, evaluation, compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### a simple k-nearest neighbour example
### datasets
## Not run: plot(x)
data(golub)
golubY <- golub[,1]
golubX <- as.matrix(golub[,-1])
### learningsets
```

```
set.seed(111)
lset <- GenerateLearningsets(y=golubY, method = "CV", fold=5, strat =TRUE)
### 1. GeneSelection
selttest <- GeneSelection(golubX, golubY, learningsets = lset, method = "t.test")
### 2. tuning
tunek <- tune(golubX, golubY, learningsets = lset, genesel = selttest, nbgene = 20, classifier = knnCMA)
### 3. classification
knn1 <- classification(golubX, golubY, learningsets = lset, genesel = selttest,
                       tuneres = tunek, nbgene = 20, classifier = knnCMA)
### steps 1.-3. combined into one step:
knn2 <- classification(golubX, golubY, learningsets = lset,
                       genesellist = list(method  = "t.test"), classifier = knnCMA,
                       tuninglist = list(grids = list(k = c(1:8))), nbgene = 20)
### show and analyze results:
knnjoin <- join(knn2)
show(knn2)
eval <- evaluation(knn2, measure = "misclassification")
show(eval)
summary(eval)
boxplot(eval)

## End(Not run)
```

`classification-methods` *General method for classification with various methods*

Description

Perform classification for the following signatures:

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult `classification`.

`cloutput-class` *"cloutput"*

Description

Object returned by one of the classifiers (functions ending with `CMA`)

Slots

`learnind`: Vector of indices that indicates which observations where used in the learning set.

`y`: Actual (true) class labels of predicted observations.

`yhat`: Predicted class labels by the classifier.

`prob`: A `numeric matrix` whose rows equals the number of predicted observations (length of `y`/`yhat`) and whose columns equal the number of different classes in the learning set. Rows add up to one. Entry `j,k` of this matrix contains the probability for the `j`-th predicted observation to belong to class `k`. Can be a matrix of `NA`s, if the classifier used does not provide any probabilities

`method`: Name of the classifer used.

`mode`: `character`, one of `"binary"` (if the number of classes in the learning set is two) or `multiclass` (if it is more than two).

`model`: List containing the constructed classifiers.

Methods

show Use `show(cloutput-object)` for brief information

ftable Use `ftable(cloutput-object)` to obtain a confusion matrix/cross-tabulation of `y` vs. `yhat`, s. `ftable,cloutput-method`.

plot Use `plot(cloutput-object)` to generate a probability plot of the matrix `prob` described above, s. `plot,cloutput-method`

roc Use `roc(cloutput-object)` to compute the empirical ROC curve and the Area Under the Curve (AUC) based on the predicted probabilities, s.`roc,cloutput-method`

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See Also

`clvarseloutput` `compBoostCMA`, `dldaCMA`, `ElasticNetCMA`, `fdaCMA`, `flexdaCMA`, `gbmCMA`, `knnCMA`, `ldaCMA`, `LassoCMA`, `nnetCMA`, `pknnCMA`, `plrCMA`, `pls_ldaCMA`, `pls_lrCMA`, `pls_rfCMA`, `pnnCMA`, `qdaCMA`, `rfCMA`, `scdaCMA`, `shrinkldaCMA`, `svmCMA`

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clvarseloutput-class *"clvarseloutput"*

Description

Object returned by all classifiers that can peform variable selection or compute variable importance. These are:

- Random Forest, s. `rfCMA`,
- Componentwise Boosting, s. `compBoostCMA`,
- LASSO-logistic regression, s. `LassoCMA`,
- ElasticNet-logistic regression, s. `ElasticNetCMA`

. Objects of class `clvarseloutput` extend both the class `cloutuput` and `varsel`, s. below.

Slots

`learnind`: Vector of indices that indicates which observations where used in the learning set.

`y`: Actual (true) class labels of predicted observations.

`yhat`: Predicted class labels by the classifier.

`prob`: A `numeric matrix` whose rows equals the number of predicted observations (length of `y`/`yhat`) and whose columns equal the number of different classes in the learning set. Rows add up to one. Entry `j,k` of this matrix contains the probability for the `j`-th predicted observation to belong to class `k`. Can be a matrix of `NA`s, if the classifier used does not provide any probabilities

`method`: Name of the classifer used.

`mode`: `character`, one of `"binary"` (if the number of classes in the learning set is two) or `multiclass` (if it is more than two).

`varsel`: `numeric` vector of variable importance measures (for Random Forest) or absolute values of regression coefficients (for the other three methods mentionned above) (from which the majority will be zero).

Extends

Class `"cloutput"`, directly. Class `"varseloutput"`, directly.

Methods

show Use `show(cloutput-object)` for brief information

ftable Use `ftable(cloutput-object)` to obtain a confusion matrix/cross-tabulation of `y` vs. `yhat`, s. `ftable,cloutput-method`.

plot Use `plot(cloutput-object)` to generate a probability plot of the matrix `prob` described above, s. `plot,cloutput-method`

roc Use `roc(cloutput-object)` to compute the empirical ROC curve and the Area Under the Curve (AUC) based on the predicted probabilities, s.`roc,cloutput-method`

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See Also

`rfCMA`, `compBoostCMA`, `LassoCMA`, `ElasticNetCMA`

---

compare *Compare different classifiers*

Description

Classifiers can be evaluated separately using the method `evaluation`. Normally, several classifiers are used for the same dataset and their performance is compared. This comparison procedure is essentially facilitated by this method. For S4 method information, s. `compare-methods`

Usage

```
compare(clresultlist, measure = c("misclassification", "sensitivity",
"specificity", "average probability", "brier score", "auc"), aggfun =
meanrm, plot = FALSE, ...)
```

Arguments

clresultlist	A list of lists (!) of objects of class cloutput or clvarseloutput. Each inner list is usually returned by classification. Additionally, the different list elements of the outer list should have been created by different classifiers, s. also example below.
measure	A character vector containing one or more of the elements listed below. By default, all measures are computed, using evaluation with scheme = "iterationwise". Note that "sensitivity", "specificity", "auc" cannot be computed for the multiclass case. "misclassification" The missclassifcation rate. "sensitivity" The sensitivity or 1-false negative rate. Can only be computed for binary classifcation. "specificity" The specificity or 1-false positive rate. Can only be computed for binary classification. "average probability" The average probability assigned to the correct class. Requirement is that the used classifier provides probability estimations. The optimum performance is 1. "brier score" The Brier Score is generally defined as <sum over all observation i> <sum over all classes k> (I(y_i=k)-P(k))^2, with I() denoting the indicator function and P(k) the estimated probability for class k. The optimum performance is 0. "auc" The Area under the Curve (AUC) belonging to the empirical ROC curve computed from the estimated probabilities and the true class labels. Can only be computed for binary classification and if "scheme = iterationwise", s. below. S. also roc,cloutput-method.
aggfun	Function that determines how performance among different iterations are aggregared. Default is meanrm, which computes the mean using na.rm=T. Other possible choices are quantiles.
plot	Should the performance of different classifiers be visualized by a joint boxplot ? Default is FALSE.
...	Further arguments passed to boxplot in the case that plot = TRUE.

Value

A data.frame with rows corresponding to the compared classifiers and columns to the performance measures, aggregated by aggfun, s. above.

Note

If more than one measure is computed and plot = TRUE, one separate plot is created for each of them.

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References

Dudoit, S., Fridlyand, J., Speed, T. P. (2002)
Comparison of discrimination methods for the classification of tumors using gene expression data. *Journal of the American Statistical Association 97, 77-87*

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

See Also

classification, evaluation

Examples

```
## Not run:
### compare the performance of several discriminant analysis methods
### for the Khan dataset:
data(khan)
khanX <- as.matrix(khan[,-1])
khanY <- khan[,1]
set.seed(27611)
fiveCV10iter <- GenerateLearningsets(y=khanY, method = "CV", fold = 5, niter = 2, strat = TRUE)
### candidate methods:  DLDA, LDA, QDA, pls_LDA, sclda
class_dlda <- classification(X = khanX, y=khanY, learningsets = fiveCV10iter, classifier = dldaCMA)
### peform GeneSlection for LDA, FDA, QDA (using F-Tests):
genesel_da <- GeneSelection(X=khanX, y=khanY, learningsets = fiveCV10iter, method = "f.test")
###
class_lda <- classification(X = khanX, y=khanY, learningsets = fiveCV10iter, classifier = ldaCMA, genesel= gene

class_qda <- classification(X = khanX, y=khanY, learningsets = fiveCV10iter, classifier = qdaCMA, genesel = gen

### We now make a comparison concerning the performance (sev. measures):
### first, collect in a list:
dalike <- list(class_dlda, class_lda, class_qda)
### use pre-defined compare function:
comparison <- compare(dalike, plot = TRUE, measure = c("misclassification", "brier score", "average probabilit
print(comparison)

## End(Not run)
```

---

compare-methods *Compare different classifiers*

Description

Compare different classifiers for the following signatures:

Methods

clresultlist = "list" signature 1

For further argument and output information, consult compare

---

compBoostCMA *Componentwise Boosting*

Description

Roughly speaking, Boosting combines 'weak learners' in a weighted manner in a stronger ensemble.

'Weak learners' here consist of linear functions in one component (variable), as proposed by Buehlmann and Yu (2003).

It also generates sparsity and can as well be as used for variable selection alone. (s. GeneSelection).

For S4 method information, see compBoostCMA-methods.

Usage

```
compBoostCMA(X, y, f, learnind, loss = c("binomial", "exp", "quadratic"), mstop = 100, nu = 0.1, mode
```

Arguments

X	Gene expression data. Can be one of the following: • A matrix. Rows correspond to observations, columns to variables. • A data.frame, when f is *not* missing (s. below). • An object of class ExpressionSet.
y	Class labels. Can be one of the following: • A numeric vector. • A factor. • A character if X is an ExpressionSet that specifies the phenotype variable. • missing, if X is a data.frame and a proper formula f is provided. **WARNING**: The class labels will be re-coded to range from 0 to K-1, where K is the total number of different classes in the learning set.
f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.
learnind	An index vector specifying the observations that belong to the learning set. May be missing; in that case, the learning set consists of all observations and predictions are made on the learning set.
loss	Character specifying the loss function - one of "binomial" (LogitBoost), "exp" (AdaBoost), "quadratic"(L2Boost).
mstop	Number of boosting iterations, i.e. number of updates to perform. The default (100) does not necessarily produce good results, therefore usage of tune for this argument is highly recommended.
nu	Shrinkage factor applied to the update steps, defaults to 0.1. In most cases, it suffices to set nu to a very low value and to concentrate on the optimization of mstop.
models	a logical value indicating whether the model object shall be returned
...	Currently unused arguments.

Details

The method is partly based on code from the package `mboost` from T. Hothorn and P. Buehlmann.

The algorithm for the multiclass case is described in Lutz and Buehlmann (2006) as 'rowwise updating'.

Value

An object of class `clvarseloutput`.

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References

Buelmann, P., Yu, B. (2003).

Boosting with the L2 loss: Regression and Classification.

Journal of the American Statistical Association, 98, 324-339

Buehlmann, P., Hothorn, T.

Boosting: A statistical perspective.

Statistical Science (to appear)

Lutz, R., Buehlmann, P. (2006).

Boosting for high-multivariate responses in high-dimensional linear regression.

Statistica Sinica 16, 471-494.

See Also

`dldaCMA`, `ElasticNetCMA`, `fdaCMA`, `flexdaCMA`, `gbmCMA`, `knnCMA`, `ldaCMA`, `LassoCMA`, `nnetCMA`, `pknnCMA`, `plrCMA`, `pls_ldaCMA`, `pls_lrCMA`, `pls_rfCMA`, `pnnCMA`, `qdaCMA`, `rfCMA`, `scdaCMA`, `shrinkldaCMA`, `svmCMA`

Examples

```
 ### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression
golubX <- as.matrix(golub[,-1])
### select learningset
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run componentwise (logit)-boosting (not tuned)
result <- compBoostCMA(X=golubX, y=golubY, learnind=learnind, mstop = 500)
### show results
show(result)
ftable(result)
plot(result)
### multiclass example:
```

```
### load Khan data
data(khan)
### extract class labels
khanY <- khan[,1]
### extract gene expression
khanX <- as.matrix(khan[,-1])
### select learningset
set.seed(111)
learnind <- sample(length(khanY), size=floor(ratio*length(khanY)))
### run componentwise multivariate (logit)-boosting (not tuned)
result <- compBoostCMA(X=khanX, y=khanY, learnind=learnind, mstop = 1000)
### show results
show(result)
ftable(result)
plot(result)
```

---

compBoostCMA-methods *Componentwise Boosting*

Description

Roughly speaking, Boosting combines 'weak learners' in a weighted manner in a stronger ensemble.

'Weak learners' here consist of linear functions in one component (variable), as proposed by Buehlmann and Yu (2003).

It also generates sparsity and can as well be as used for variable selection alone. (s. GeneSelection.)

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult compBoostCMA.

---

dldaCMA *Diagonal Discriminant Analysis*

Description

Performs a diagonal discriminant analysis under the assumption of a multivariate normal distribution in each classes (with equal, diagonally structured) covariance matrices. The method is also known under the name 'naive Bayes' classifier.

For S4 method information, see dldaCMA-methods.

Usage

```
dldaCMA(X, y, f, learnind, models=FALSE, ...)
```

Arguments

X	Gene expression data. Can be one of the following: • A matrix. Rows correspond to observations, columns to variables. • A data.frame, when f is *not* missing (s. below). • An object of class ExpressionSet.
y	Class labels. Can be one of the following: • A numeric vector. • A factor. • A character if X is an ExpressionSet that specifies the phenotype variable. • missing, if X is a data.frame and a proper formula f is provided. **WARNING**: The class labels will be re-coded to range from 0 to K-1, where K is the total number of different classes in the learning set.
f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.
learnind	An index vector specifying the observations that belong to the learning set. May be missing; in that case, the learning set consists of all observations and predictions are made on the learning set.
models	a logical value indicating whether the model object shall be returned
...	Currently unused argument.

Value

An object of class cloutput.

Note

As opposed to linear or quadratic discriminant analysis, variable selection is not strictly necessary.

Author(s)

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References

McLachlan, G.J. (1992).

Discriminant Analysis and Statistical Pattern Recognition.

Wiley, New York

See Also

compBoostCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression
golubX <- as.matrix(golub[,-1])
### select learningset
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run DLDA
dldaresult <- dldaCMA(X=golubX, y=golubY, learnind=learnind)
### show results
show(dldaresult)
ftable(dldaresult)
plot(dldaresult)
### multiclass example:
### load Khan data
data(khan)
### extract class labels
khanY <- khan[,1]
### extract gene expression
khanX <- as.matrix(khan[,-1])
### select learningset
set.seed(111)
learnind <- sample(length(khanY), size=floor(ratio*length(khanY)))
### run LDA
ldaresult <- dldaCMA(X=khanX, y=khanY, learnind=learnind)
### show results
show(dldaresult)
ftable(dldaresult)
plot(dldaresult)
```

---

dldaCMA-methods *Diagonal Discriminant Analysis*

Description

Performs a diagonal discriminant analysis under the assumption of a multivariate normal distribution in each classes (with equal, diagonally structured) covariance matrices. The method is also known under the name 'naive Bayes' classifier.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult dldaCMA.

ElasticNetCMA *Classfication and variable selection by the ElasticNet*

Description

Zou and Hastie (2004) proposed a combined L1/L2 penalty for regularization and variable selection. The Elastic Net penalty encourages a grouping effect, where strongly correlated predictors tend to be in or out of the model together. The computation is done with the function `glmpath` from the package of the same name.
The method can be used for variable selection alone, s. `GeneSelection`.
For `S4` method information, see `ElasticNetCMA-methods`.

Usage

```
ElasticNetCMA(X, y, f, learnind, norm.fraction = 0.1, alpha=0.5, models=FALSE, ...)
```

Arguments

`X`	Gene expression data. Can be one of the following: • A `matrix`. Rows correspond to observations, columns to variables. • A `data.frame`, when `f` is *not* missing (s. below). • An object of class `ExpressionSet`. **note**: by default, the predictors are scaled to have unit variance and zero mean. Can be changed by passing `standardize = FALSE` via the `...` argument.
`y`	Class labels. Can be one of the following: • A `numeric` vector. • A `factor`. • A `character` if `X` is an `ExpressionSet` that specifies the phenotype variable. • `missing`, if `X` is a `data.frame` and a proper formula `f` is provided. **WARNING**: The class labels will be re-coded to range from `0` to `K-1`, where `K` is the total number of different classes in the learning set.
`f`	A two-sided formula, if `X` is a `data.frame`. The left part correspond to class labels, the right to variables.
`learnind`	An index vector specifying the observations that belong to the learning set. May be `missing`; in that case, the learning set consists of all observations and predictions are made on the learning set.
`norm.fraction`	L1 Shrinkage intensity, expressed as the fraction of the coefficient L1 norm compared to the maximum possible L1 norm (corresponds to `fraction = 1`). Lower values correspond to higher shrinkage. Note that the default (0.1) need not produce good results, i.e. tuning of this parameter is recommended.
`alpha`	The elasticnet mixing parameter, with 0<alpha<= 1. The penalty is defined as (1-alpha)/2||beta|_2^2+alpha|beta|_1. `alpha=1` is the lasso penalty; Currently 'alpha<0.01' not reliable, unless you supply your own `lambda` sequence
`models`	a logical value indicating whether the model object shall be returned
`...`	Further arguments passed to the function `glmpath` from the package of the same name.

Value

An object of class clvarseloutput.

Note

For a strongly related method, s. LassoCMA.
Up to now, this method can only be applied to binary classification.

Author(s)

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References

Zhou, H., Hastie, T. (2004).
Regularization and variable selection via the elastic net. *Journal of the Royal Statistical Society B, 67(2),301-320*

Young-Park, M., Hastie, T. (2007)
L1-regularization path algorithm for generalized linear models.
Journal of the Royal Statistical Society B, 69(4), 659-677

See Also

compBoostCMA, dldaCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression
golubX <- as.matrix(golub[,-1])
### select learningset
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run ElasticNet - penalized logistic regression (no tuning)
result <- ElasticNetCMA(X=golubX, y=golubY, learnind=learnind, norm.fraction = 0.2, alpha=0.5)
show(result)
ftable(result)
plot(result)
```

ElasticNetCMA-methods *Classfication and variable selection by the ElasticNet*

Description

Zou and Hastie (2004) proposed a combined L1/L2 penalty for regularization and variable selection. The Elastic Net penalty encourages a grouping effect, where strongly correlated predictors tend to be in or out of the model together. The computation is done with the function `glmpath` from the package of the same name.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For references, further argument and output information, consult `ElasticNetCMA`

evaloutput-class *"evaloutput"*

Description

Object returned by the method `evaluation`.

Slots

`score`**:** A numeric vector of performance scores whose length depends on `"scheme"`, s.below. It equals the number of iterations (number of different datasets) if `"scheme = iterationwise"` and the number of all observations in the complete dataset otherwise. As not necessarily all observation must be predicted at least one time, `score` can also contain `NA`s for those observations not classified at all.

`measure`**:** performance measure used, s. `evaluation`.

`scheme`**:** scheme used, s. `evaluation`

`method`**:** name of the classifier that has been evaluated.

Methods

show Use `show(evaloutput-object)` for brief information.

summary Use `summary(evaloutput-object)` to apply the classic `summary()` function to the slot `score`, s. `summary,evaloutput-method`

boxplot Use `boxplot(evaloutput-object)` to display a boxplot of the slot `score`, s. `boxplot,evaloutput-method`.

obsinfo Use `obsinfo(evaloutput-object, threshold)` to display all observations consistenly correctly or incorrectly classified (depending on the value of the argument `threshold`), s. `obsinfo`.

Author(s)

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See Also

evaluation

---

evaluation *Evaluation of classifiers*

Description

The performance of classifiers can be evaluted by six different measures and two different schemes that are described more precisely below.
For S4 method information, s. evaluation-methods.

Usage

```
evaluation(clresult, cltrain = NULL, cost = NULL, y = NULL, measure = c("misclassification", "sensit
                    scheme = c("iterationwise", "observationwise", "classwise"))
```

Arguments

clresult	A list of objects of class cloutput or clvarseloutput
cltrain	An object of class cloutput in which the *whole* dataset was used as learning set. Only used if method = "0.632" or method = "0.632+" in order to obtain an estimation for the resubsitution error rate.
cost	An optional cost matrix used if measure = "misclassification". If it is not specified (default), the cost is the usual indicator loss. Otherwise, entry i,j of cost quantifies the loss when the true class is class i-1 and the predicted class is j-1, provided the conventional coding 0,...,K-1 in the case of K classes is used. Usually, the matrix contains only non-negative entries with zeros on the diagonal, but this is not obligatory. Make sure that the dimension of the matrix matches the number of classes.
y	A vector containing the true class labels. Only needed if scheme = "classwise".
measure	Peformance measure to be used: "misclassification" The missclassifcation rate. "sensitivity" The sensitivity or 1-false negative rate. Can only be computed for binary classifcation. "specificity" The specificity or 1-false positive rate. Can only be computed for binary classification. "average probability" The average probability assigned to the correct class. Requirement is that the used classifier provides probability estimations. The optimum performance is 1. "brier score" The Brier Score is generally defined as <sum over all observation i> <sum over all classes k> (I(y_i=k)-P(k))^2, with I() denoting the indicator function and P(k) the estimated probability for class k. The optimum performance is 0.

"auc" The Area under the Curve (AUC) belonging to the empirical ROC curve computed from the estimated probabilities and the true class labels. Can only be computed for binary classification and if "scheme = iterationwise", s. below. S. also roc,cloutput-method.

"0.632" The 0.632 estimator (s. reference) for the misclassification rate (applied iteration- or) observationwise, if bootstrap learning sets have been used. Note that cltrain must be provided.

"0.632+" The 0.632+ estimator (s. reference) for the misclassification rate (applied iteration- or) observationwise, if bootstrap learning sets have been used. Note that cltrain must be provided.

scheme

"iterationwise" The performance measures listed above are computed for each different iteration, i.e. each different learningset

"observationwise" The performance measures listed above (except for "auc") are computed separately for each observation classified one or several times, depending on the learningset scheme.

"classwise" The performance measures (exceptions: "auc", "0.632", "0.632+") are computed separately for each class, averaged over both iterations and observations.

Value

An object of class evaloutput.

Author(s)

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Christoph Bernau <bernau@ibe.med.uni-muenchen.de>

References

Efron, B. and Tibshirani, R. (1997). Improvements on cross-validation: The .632+ bootstrap method.
Journal of the American Statistical Association, 92, 548-560.

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

See Also

evaloutput, classification, compare

Examples

```
### simple linear discriminant analysis example using bootstrap datasets:
### datasets:
data(golub)
golubY <- golub[,1]
### extract gene expression from first 10 genes
golubX <- as.matrix(golub[,2:11])
### generate 25 bootstrap datasets
set.seed(333)
bootds <- GenerateLearningsets(y = golubY, method = "bootstrap", ntrain = 30, niter = 10, strat = TRUE)
```

```
### run classification()
ldalist <- classification(X=golubX, y=golubY, learningsets = bootds, classifier=ldaCMA)
### Evaluation:
eval_iter <- evaluation(ldalist, scheme = "iter")
eval_obs <- evaluation(ldalist, scheme = "obs")
show(eval_iter)
show(eval_obs)
summary(eval_iter)
summary(eval_obs)
### auc with boxplot
eval_auc <- evaluation(ldalist, scheme = "iter", measure = "auc")
boxplot(eval_auc)
### which observations have often been misclassified ?
obsinfo(eval_obs, threshold = 0.75)
```

`evaluation-methods` *Evaluation of classifiers*

Description

Evaluate classifiers for the following signatures:

Methods

clresult = "list" signature 1

For further argument and output information, consult `evaluation`.

`fdaCMA` *Fisher's Linear Discriminant Analysis*

Description

Fisher's Linear Discriminant Analysis constructs a subspace of 'optimal projections' in which classification is performed. The directions of optimal projections are computed by the function `cancor` from the package `stats`. For an exhaustive treatment, see e.g. Ripley (1996).

For `S4` method information, see `fdaCMA-methods`.

Usage

```
fdaCMA(X, y, f, learnind, comp = 1, plot = FALSE,models=FALSE)
```

Arguments

`X`	Gene expression data. Can be one of the following: • A `matrix`. Rows correspond to observations, columns to variables. • A `data.frame`, when `f` is *not* missing (s. below). • An object of class `ExpressionSet`.
`y`	Class labels. Can be one of the following: • A `numeric` vector.

- A factor.
- A character if X is an ExpressionSet that specifies the phenotype variable.
- missing, if X is a data.frame and a proper formula f is provided. **WARNING**: The class labels will be re-coded to range from 0 to K-1, where K is the total number of different classes in the learning set.

f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.
learnind	An index vector specifying the observations that belong to the learning set. May be missing; in that case, the learning set consists of all observations and predictions are made on the learning set.
comp	Number of discriminant coordinates (projections) to compute. Default is one, must be smaller than or equal to K-1, where K is the number of classes.
plot	Should the projections onto the space spanned by the optimal projection directions be plotted ? Default is FALSE.
models	a logical value indicating whether the model object shall be returned

Value

An object of class cloutput.

Note

Excessive variable selection has usually to performed before fdaCMA can be applied in the p > n setting. Not reducing the number of variables can result in an error message.

Author(s)

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Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Ripley, B.D. (1996)

Pattern Recognition and Neural Networks.

Cambridge University Press

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression from first 10 genes
golubX <- as.matrix(golub[,2:11])
### select learningset
```

```
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run FDA
fdaresult <- fdaCMA(X=golubX, y=golubY, learnind=learnind, comp = 1, plot = TRUE)
### show results
show(fdaresult)
ftable(fdaresult)
plot(fdaresult)
### multiclass example:
### load Khan data
data(khan)
### extract class labels
khanY <- khan[,1]
### extract gene expression from first 10 genes
khanX <- as.matrix(khan[,2:11])
### select learningset
set.seed(111)
learnind <- sample(length(khanY), size=floor(ratio*length(khanY)))
### run FDA
fdaresult <- fdaCMA(X=khanX, y=khanY, learnind=learnind, comp = 2, plot = TRUE)
### show results
show(fdaresult)
ftable(fdaresult)
plot(fdaresult)
```

`fdaCMA-methods` *Fisher's Linear Discriminant Analysis*

Description

Fisher's Linear Discriminant Analysis constructs a subspace of 'optimal projections' in which classification is performed. The directions of optimal projections are computed by the function `cancor` from the package `stats`. For an exhaustive treatment, see e.g. Ripley (1996).

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For references, further argument and output information, consult `fdaCMA`.

filter — *Filter functions for Gene Selection*

Description

The functions listed above are usually not called by the user but via GeneSelection.

Usage

```
ttest(X, y, learnind, ...)
welchtest(X, y, learnind, ...)
ftest(X, y, learnind,...)
kruskaltest(X, y, learnind,...)
limmatest(X, y, learnind,...)
golubcrit(X, y, learnind,...)
rfe(X, y, learnind,...)
shrinkcat(X,y,learnind,...)
```

Arguments

X	A numeric matrix of gene expression values.
y	A numeric vector of class labels.
learnind	An index vector specifying the observations that belong to the learning set.
...	Currently unused argument.

Value

An object of class varseloutput.

References

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

flexdaCMA — *Flexible Discriminant Analysis*

Description

This method is experimental.

It is easy to show that, after appropriate scaling of the predictor matrix X, Fisher's Linear Discriminant Analysis is equivalent to Discriminant Analysis in the space of the fitted values from the linear regression of the nlearn x K indicator matrix of the class labels on X. This gives rise to 'nonlinear discrimant analysis' methods that expand X in a suitable, more flexible basis. In order to avoid overfitting, penalization is used. In the implemented version, the linear model is replaced by a generalized additive one, using the package mgcv.

For S4 method information, s. flexdaCMA-methods.

Usage

```
flexdaCMA(X, y, f, learnind, comp = 1, plot = FALSE, models=FALSE, ...)
```

Arguments

X	Gene expression data. Can be one of the following: • A matrix. Rows correspond to observations, columns to variables. • A data.frame, when f is *not* missing (s. below). • An object of class ExpressionSet.
y	Class labels. Can be one of the following: • A numeric vector. • A factor. • A character if X is an ExpressionSet that specifies the phenotype variable. • missing, if X is a data.frame and a proper formula f is provided. **WARNING**: The class labels will be re-coded to range from 0 to K-1, where K is the total number of different classes in the learning set.
f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.
learnind	An index vector specifying the observations that belong to the learning set. May be missing; in that case, the learning set consists of all observations and predictions are made on the learning set.
comp	Number of discriminant coordinates (projections) to compute. Default is one, must be smaller than or equal to K-1, where K is the number of classes.
plot	Should the projections onto the space spanned by the optimal projection directions be plotted ? Default is FALSE.
models	a logical value indicating whether the model object shall be returned
...	Further arguments passed to the function gam from the package mgcv.

Value

An object of class cloutput.

Note

Excessive variable selection has usually to performed before flexdaCMA can be applied in the p > n setting. Recall that the original predictor dimension is even enlarged, therefore, it should be applied only with very few variables.

Author(s)

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Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Ripley, B.D. (1996)

Pattern Recognition and Neural Networks.

Cambridge University Press

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression from first 5 genes
golubX <- as.matrix(golub[,2:6])
### select learningset
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run flexible Discriminant Analysis
result <- flexdaCMA(X=golubX, y=golubY, learnind=learnind, comp = 1)
### show results
show(result)
ftable(result)
plot(result)
```

---

flexdaCMA-methods *Flexible Discriminant Analysis*

Description

This method is experimental.

It is easy to show that, after appropriate scaling of the predictor matrix X, Fisher's Linear Discriminant Analysis is equivalent to Discriminant Analysis in the space of the fitted values from the linear regression of the nlearn x K indicator matrix of the class labels on X. This gives rise to 'nonlinear discrimant analysis' methods that expand X in a suitable, more flexible basis. In order to avoid overfitting, penalization is used. In the implemented version, the linear model is replaced by a generalized additive one, using the package mgcv.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult flexdaCMA.

ftable *Cross-tabulation of predicted and true class labels*

Description

An object of class cloutput contains (among others) the slot y and yhat. The former contains the true, the last the predicted class labels. Both are cross-tabulated in order to obtain a so-called confusion matrix. Counts out of the diagonal are misclassifications.

Arguments

x	An object of class cloutput
...	Currently unused argument.

Value

No return.

Author(s)

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Anne-Laure Boulesteix http://www.slcmsr.net/boulesteix

See Also

For more advanced evaluation: evaluation

gbmCMA *Tree-based Gradient Boosting*

Description

Roughly speaking, Boosting combines 'weak learners' in a weighted manner in a stronger ensemble. This method calls the function gbm.fit from the package gbm. The 'weak learners' are simple trees that need only very few splits (default: 1).

For S4 method information, see gbmCMA-methods.

Usage

```
gbmCMA(X, y, f, learnind, models=FALSE,...)
```

Arguments

X	Gene expression data. Can be one of the following: • A matrix. Rows correspond to observations, columns to variables. • A data.frame, when f is *not* missing (s. below). • An object of class ExpressionSet.
y	Class labels. Can be one of the following: • A numeric vector. • A factor. • A character if X is an ExpressionSet that specifies the phenotype variable. • missing, if X is a data.frame and a proper formula f is provided. **WARNING**: The class labels will be re-coded to range from 0 to K-1, where K is the total number of different classes in the learning set.
f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.
learnind	An index vector specifying the observations that belong to the learning set. May be missing; in that case, the learning set consists of all observations and predictions are made on the learning set.
models	a logical value indicating whether the model object shall be returned
...	Further arguments passed to the function gbm.fit from the package of the same name. Worth mentionning are ntrees Number of trees to fit (size of the ensemble), defaults to 100. This parameter should be optimized using tune. shrinkage The learning rate (default is 0.001). Usually fixed to a very low value. distribution Loss function to be used. Default is "bernoulli", i.e. LogitBoost, a (less robust) alternative is "adaboost". interaction.depth Number of splits used by the 'weak learner' (single decision tree). Default is 1.

Value

An onject of class cloutput.

Note

Up to now, this method can only be applied to binary classification.

Author(s)

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References

Ridgeway, G. (1999).

The state of boosting.

Computing Science and Statistics, 31:172-181

Friedman, J. (2001).

Greedy Function Approximation: A Gradient Boosting Machine.

Annals of Statistics 29(5):1189-1232.

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression
golubX <- as.matrix(golub[,-1])
### select learningset
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run tree-based gradient boosting (no tuning)
gbmresult <- gbmCMA(X=golubX, y=golubY, learnind=learnind, n.trees = 500)
show(gbmresult)
ftable(gbmresult)
plot(gbmresult)
```

---

gbmCMA-methods *Tree-based Gradient Boosting*

Description

Roughly speaking, Boosting combines 'weak learners' in a weighted manner in a stronger ensemble. This method calls the function `gbm.fit` from the package gbm. The 'weak learners' are simple trees that need only very few splits (default: 1).

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult gbmCMA.

GenerateLearningsets *Repeated Divisions into learn- and tets sets*

Description

Due to very small sample sizes, the classical division learnset/testset does not give accurate information about the classification performance. Therefore, several different divisions should be used and aggregated. The implemented methods are discussed in Braga-Neto and Dougherty (2003) and Molinaro et al. (2005) whose terminology is adopted.

This function is usually the basis for all deeper analyses.

Usage

```
GenerateLearningsets(n, y, method = c("LOOCV", "CV", "MCCV", "bootstrap"),
                     fold = NULL, niter = NULL, ntrain = NULL, strat = FALSE)
```

Arguments

n	The total number of observations in the available data set. May be missing if y is provided instead.
y	A vector of class labels, either numeric or a factor. *Must* be given if strat=TRUE or n is not specified.
method	Which kind of scheme should be used to generate divisions into learning sets and test sets ? Can be one of the following: **"LOOCV"** Leaving-One-Out Cross Validation. **"CV"** (Ordinary) Cross-Validation. Note that fold must as well be specified. **"MCCV"** Monte-Carlo Cross Validation, i.e. random divisions into learning sets with ntrain(s.below) observations and tests sets with ntrain observations. **"bootstrap"** Learning sets are generated by drawing n times with replacement from all observations. Those not drawn not all form the test set.
fold	Gives the number of CV-groups. Used only when method="CV"
niter	Number of iterations (s.details).
ntrain	Number of observations in the learning sets. Used only when method="MCCV".
strat	Logical. Should stratified sampling be performed, i.e. the proportion of observations from each class in the learning sets be the same as in the whole data set ? Does not apply for method = "LOOCV".

Details

- When method="CV", niter gives the number of times the whole CV-procedure is repeated. The output matrix has then foldxniter rows. When method="MCCV" or method="bootstrap", niter is simply the number of considered learning sets.
- Note that method="CV",fold=n is equivalent to method="LOOCV".

Value

An object of class learningsets

Author(s)

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References

Braga-Neto, U.M., Dougherty, E.R. (2003).

Is cross-validation valid for small-sample microarray classification ?

Bioinformatics, 20(3), 374-380

Molinaro, A.M., Simon, R., Pfeiffer, R.M. (2005).

Prediction error estimation: a comparison of resampling methods.

Bioinformatics, 21(15), 3301-3307

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

See Also

learningsets, GeneSelection, tune, classification

Examples

```
# LOOCV
loo <- GenerateLearningsets(n=40, method="LOOCV")
show(loo)
# five-fold-CV
CV5 <- GenerateLearningsets(n=40, method="CV", fold=5)
show(loo)
# MCCV
mccv <- GenerateLearningsets(n=40, method = "MCCV", niter=3, ntrain=30)
show(mccv)
# Bootstrap
boot <- GenerateLearningsets(n=40, method="bootstrap", niter=3)
# stratified five-fold-CV
set.seed(113)
classlabels <- sample(1:3, size = 50, replace = TRUE, prob = c(0.3, 0.5, 0.2))
CV5strat <- GenerateLearningsets(y = classlabels, method="CV", fold=5, strat = TRUE)
show(CV5strat)
```

---

genesel-class *"genesel"*

Description

Object returned from a call to GeneSelection

Slots

`rankings`: A list of matrices. For the two-class case and the multi-class case where a genuine multi-class method has been used for variable selection, the length of the list is one. Otherwise, it is named according to the different binary scenarios (e.g. `1 vs 3`). Each list element is a `matrix` with rows corresponding to iterations (different `learningsets`) and columns to variables. Each row thus contains an index vector representing the order of the variables with respect to their variable importance (s. slot `importance`)

`importance`: A list of matrices, with the same structure as described for the slot `rankings`. Each row of these matrices are ordered according to `rankings` and contain the variable importance measure (absolute value of test statistic or regression coefficient).

`method`: Name of the method used for variable selection, s. `GeneSelection`.

`scheme`: The scheme used in the case of a non-binary response, one of `"pairwise"`, `"one-vs-all"` or `"multiclass"`.

Methods

show Use `show(genesel-object)` for brief information

toplist Use `toplist(genesel-object, k=10, iter = 1)` to display the top first 10 variables and their variable importance for the first iteration (first learningset), s.`toplist`.

plot Use `plot(genesel-object, k=10, iter=1)` to display a barplot of the variable importance of the top first 10 variables, s. `plot,genesel-method`

Author(s)

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See Also

`GeneSelection`

`GeneSelection` *General method for variable selection with various methods*

Description

For different learning data sets as defined by the argument `learningsets`, this method ranks the genes from the most relevant to the less relevant using one of various 'filter' criteria or provides a sparse collection of variables (Lasso, ElasticNet, Boosting). The results are typically used for variable selection for the classification procedure that follows.
For S4 class information, s. `GeneSelection-methods`.

Usage

```
GeneSelection(X, y, f, learningsets, method = c("t.test", "welch.test", "wilcox.test", "f.test", "k
```

Arguments

X	Gene expression data. Can be one of the following: • A matrix. Rows correspond to observations, columns to variables. • A data.frame, when f is *not* missing (s. below). • An object of class ExpressionSet.
y	Class labels. Can be one of the following: • A numeric vector. • A factor. • A character if X is an ExpressionSet. • missing, if X is a data.frame and a proper formula f is provided.
f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.
learningsets	An object of class learningsets. May be missing, then the complete datasets is used as learning set.
method	A character specifying the method to be used: t.test two-sample t.test (equal variances for both classes assumed). welch.test Welch modification of the t.test (unequal variances for both classes). wilcox.test Wilcoxon rank sum test. f.test F test belonging to the linear hypothesis that the mean is the same for all classes. Usually used for the multiclass scheme, is equivalent to method = t.test in the two-class case. kruskal.test Multi-class generalization of the Wilcoxon rank sum test and the nonparametric pendant to the F test, respectively. limma 'Moderated t' statistic for the two-class case and 'moderated F' statistic for the multiclass case, described in Smyth (2003). Requires the package limma. rfe One-step Recursive Feature Elimination, based on the Support Vector Machine. The method is decribed in Guyon et al. (2002). Requires the package e1071. Take care that appropriate hyperparameters are passed by the ... argument. rf Random Forest Variable Importance Measure. Requires the package randomForest lasso L1 penalized logistic regression leads to sparsity with respect to the variables used. Calls the function LassoCMA, which requires the package glmpath. **warning**: Take care that appropriate hyperparameters are passed by the ... argument. elasticnet Penalized logistic regression with both L1 and L2 penalty, claimed by Zhou and Hastie (2004) to select 'variable groups'. Calls the function ElasticNetCMA, which requires the package glmpath. **warning**: Take care that appropriate hyperparameters are passed by the ... argument. boosting Componentwise boosting (Buehlmann and Yu, 2003) has been shown to mimic the LASSO (Efron et al., 2004; Buehlmann and Yu, 2006). Calls the function compBoostCMA Take care that appropriate hyperparameters are passed by the ... argument. golub The (theoretically unfounded) variable selection criterion used by Golub et al. (1999), s. golub. shrinkcat The correlation-adjusted t-score from Zuber and Strimmer (2009)

scheme	The scheme to be used in the case of a non-binary response. Must be one of "pairwise","one-vs-all" or "multiclass". The last case only makes sense if method is one of f.test, limma, rf, boosting, which can directly be applied to the multi class case.
trace	Should the progress be traced ? Default is TRUE.
...	Further arguments passed to the function performing variable selection, s. method.

Value

An object of class genesel.

Note

most of the methods described above are only apt for the binary classification case. The only ones that can be used without restriction in the multiclass case are

- f.test
- kruskal.test
- rf
- boosting

For the rest, pairwise or one-vs-all schemes are used.

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References

Smyth, G. K., Yang, Y.-H., Speed, T. P. (2003).
Statistical issues in microarray data analysis.
Methods in Molecular Biology 224, 111-136.

Guyon, I., Weston, J., Barnhill, S., Vapnik, V. (2002).
Gene Selection for Cancer Classification using support vector machines. *Journal of Machine Learning Research, 46, 389-422*

Zhou, H., Hastie, T. (2004).
Regularization and variable selection via the elastic net. *Journal of the Royal Statistical Society B, 67(2),301-320*

Buelmann, P., Yu, B. (2003).
Boosting with the L2 loss: Regression and Classification.
Journal of the American Statistical Association, 98, 324-339

Efron, B., Hastie, T., Johnstone, I., Tibshirani, R. (2004).
Least Angle Regression.
Annals of Statistics, 32:407-499

Buehlmann, P., Yu, B. (2006).
Sparse Boosting.
Journal of Machine Learning Research, 7- 1001:1024

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

See Also

filter, GenerateLearningsets, tune, classification

Examples

```
# load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression from first 10 genes
golubX <- as.matrix(golub[,-1])
### Generate five different learningsets
set.seed(111)
five <- GenerateLearningsets(y=golubY, method = "CV", fold = 5, strat = TRUE)
### simple t-test:
selttest <- GeneSelection(golubX, golubY, learningsets = five, method = "t.test")
### show result:
show(selttest)
toplist(selttest, k = 10, iter = 1)
plot(selttest, iter = 1)
```

GeneSelection-methods *General method for variable selection with various methods*

Description

Performs gene selection for the following signatures:

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult GeneSelection.

---

golub *ALL/AML dataset of Golub et al. (1999)*

Description

s. below

Usage

```
data(golub)
```

Format

A data frame with 38 observations and 3052 variables. The first column (named `golub.cl`) contains the tumor classes (ALL = acute lymphatic leukaemia, AML = acute myeloid leukaemia).\ `golub.cl`: a factor with levels `ALL AML`.\ `X2-X3051`: Gene expression values.

Source

Adopted from the dataset in the package `multtest`.

References

Golub, T., Slonim, D. K., Tamayo, P., Huard, C., Gaasenbeek, M., Mesirov, J. P.,

Coller, H., Loh, M. L., Downing, J., Caligiuri, M. A., Bloomfeld, C. D., Lander, E. S. (1999).

Molecular classification of cancer: class discovery and class prediction by gene expression monitoring.

Science 286, 531-537.

Examples

```
data(golub)
```

`internals` *Internal functions*

Description

Not intended to be called directly by the user.

`join` *Combine list elements returned by the method classification*

Description

The method `classification` returns a list of class `cloutput` or `clvarseloutput`. It is often more convenient to work with an object of class `cloutput` instead with a whole list, e.g. because the convenience method defined for that class can be used.

For S4 method information, s. `join-methods`

Usage

```
join(cloutputlist)
```

Arguments

`cloutputlist`	A list of objects of classes `cloutput` or `clvarseloutput`, usually that returned by a call to the method `classification`. The only requirement for a succesful join is that the used dataset and classfier are the same for each list element.

Value

An object of class cloutput. **warning:**If the elements of cloutputlist have originally been of class clvarseloutput, the slot varsel will be dropped !

Note

The result of the join method is incompatible with the methods evaluation, compare. These require the lists returned by classification.

See Also

classification, evaluation

---

join-methods *Combine list elements returned by the method classification*

Description

The list of objects of class cloutput can be unified into one object for the following signatures:

Methods

cloutputlist = "list" signature 1

For further argument and output information, consult join.

---

khan *Small blue round cell tumor dataset of Khan et al. (2001)*

Description

s. below

Usage

```
data(khan)
```

Format

A data frame with 63 observations on the following 2309 variables. The first column (named khanY) contains the tumor classes (BL = Burkitt Lymphoma, EWS = Ewing Sarcoma, NB = Neuro Blastoma, RMS = Rhabdomyosarcoma).\ khanY: a factor with levels BL EWS NB RMS \ X2-X2309: Gene expression values.

Source

Adopted from the dataset in the package pamr.

References

Khan, J., Wei, J. S., Ringner, M., Saal, L. H., Ladanyi, M., Westermann, F., Berthold, F., Schwab, M., Antonescu, C. R., Peterson, C., Meltzer, P. S., (2001).

Classification and diagnostic prediction of cancers using gene expression profiling and artificial neural networks.

Nature Medicine 7, 673-679.

Examples

```
data(khan)
```

---

knnCMA *Nearest Neighbours*

Description

Ordinary k nearest neighbours algorithm from the very fast implementation in the package `class`.

For `S4` method information, see knnCMA-methods.

Usage

```
knnCMA(X, y, f, learnind, models=FALSE, ...)
```

Arguments

`X`	Gene expression data. Can be one of the following: • A `matrix`. Rows correspond to observations, columns to variables. • A `data.frame`, when `f` is *not* missing (s. below). • An object of class `ExpressionSet`.
`y`	Class labels. Can be one of the following: • A `numeric` vector. • A `factor`. • A `character` if `X` is an `ExpressionSet` that specifies the phenotype variable. • `missing`, if `X` is a `data.frame` and a proper formula `f` is provided. **WARNING**: The class labels will be re-coded to range from `0` to `K-1`, where `K` is the total number of different classes in the learning set.
`f`	A two-sided formula, if `X` is a `data.frame`. The left part correspond to class labels, the right to variables.
`learnind`	An index vector specifying the observations that belong to the learning set. Must not be missing for this method.
`models`	a logical value indicating whether the model object shall be returned
`...`	Further arguments to be passed to `knn` from the package `class`, in particular the number of nearest neighbours to use (argument `k`).

Value

An object of class `cloutput`.

Note

Class probabilities are *not* returned. For a probabilistic variant of knn, s. pknnCMA.

Author(s)

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Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Ripley, B.D. (1996)

Pattern Recognition and Neural Networks.

Cambridge University Press

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression from first 10 genes
golubX <- as.matrix(golub[,-1])
### select learningset
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run k-nearest neighbours
result <- knnCMA(X=golubX, y=golubY, learnind=learnind, k = 3)
### show results
show(result)
ftable(result)
### multiclass example:
### load Khan data
data(khan)
### extract class labels
khanY <- khan[,1]
### extract gene expression
khanX <- as.matrix(khan[,-1])
### select learningset
set.seed(111)
learnind <- sample(length(khanY), size=floor(ratio*length(khanY)))
### run knn
result <- knnCMA(X=khanX, y=khanY, learnind=learnind, k = 5)
### show results
show(result)
ftable(result)
```

knnCMA-methods *Nearest Neighbours*

Description

Ordinary k nearest neighbours algorithm from the very fast implementation in the package class

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult knnCMA.

LassoCMA *L1 penalized logistic regression*

Description

The Lasso (Tibshirani, 1996) is one of the most popular tools for simultaneous shrinkage and variable selection. Recently, Friedman, Hastie and Tibshirani (2008) have developped and algorithm to compute the entire solution path of the Lasso for an arbitrary generalized linear model, implemented in the package glmnet. The method can be used for variable selection alone, s. GeneSelection. For S4 method information, see LassoCMA-methods.

Usage

```
LassoCMA(X, y, f, learnind, norm.fraction = 0.1,models=FALSE,...)
```

Arguments

X	Gene expression data. Can be one of the following: • A matrix. Rows correspond to observations, columns to variables. • A data.frame, when f is *not* missing (s. below). • An object of class ExpressionSet. **note**: by default, the predictors are scaled to have unit variance and zero mean. Can be changed by passing standardize = FALSE via the ... argument.
y	Class labels. Can be one of the following: • A numeric vector. • A factor. • A character if X is an ExpressionSet that specifies the phenotype variable. • missing, if X is a data.frame and a proper formula f is provided. **WARNING**: The class labels will be re-coded to range from 0 to K-1, where K is the total number of different classes in the learning set.

f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.
learnind	An index vector specifying the observations that belong to the learning set. May be missing; in that case, the learning set consists of all observations and predictions are made on the learning set.
norm.fraction	L1 Shrinkage intensity, expressed as the fraction of the coefficient L1 norm compared to the maximum possible L1 norm (corresponds to fraction = 1). Lower values correspond to higher shrinkage. Note that the default (0.1) need not produce good results, i.e. tuning of this parameter is recommended.
models	a logical value indicating whether the model object shall be returned
...	Further arguments passed to the function glmpath from the package of the same name.

Value

An object of class clvarseloutput.

Note

For a strongly related method, s. ElasticNetCMA.
Up to now, this method can only be applied to binary classification.

Author(s)

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Christoph Bernau <bernau@ibe.med.uni-muenchen.de>

References

Tibshirani, R. (1996)
Regression shrinkage and selection via the lasso.
Journal of the Royal Statistical Society B, 58(1), 267-288

Friedman, J., Hastie, T. and Tibshirani, R. (2008) Regularization
Paths for Generalized Linear Models via Coordinate Descent
http://www-stat.stanford.edu/~hastie/Papers/glmnet.pdf

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression
golubX <- as.matrix(golub[,-1])
### select learningset
ratio <- 2/3
```

```
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run L1 penalized logistic regression (no tuning)
lassoresult <- LassoCMA(X=golubX, y=golubY, learnind=learnind, norm.fraction = 0.2)
show(lassoresult)
ftable(lassoresult)
plot(lassoresult)
```

LassoCMA-methods *L1 penalized logistic regression*

Description

The Lasso (Tibshirani, 1996) is one of the most popular tools for simultaneous shrinkage and variable selection. Recently, Friedman, Hastie and Tibshirani (2008) have developped and algorithm to compute the entire solution path of the Lasso for an arbitrary generalized linear model, implemented in the package `glmnet`. The method can be used for variable selection alone, s. `GeneSelection`

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For references, further argument and output information, consult `LassoCMA`.

---

ldaCMA *Linear Discriminant Analysis*

Description

Performs a linear discriminant analysis under the assumption of a multivariate normal distribution in each classes (with equal, but generally structured) covariance matrices. The function `lda` from the package `MASS` is called for computation.

For `S4` method information, see ldaCMA-methods.

Usage

```
ldaCMA(X, y, f, learnind, models=FALSE, ...)
```

Arguments

`X`	Gene expression data. Can be one of the following: • A `matrix`. Rows correspond to observations, columns to variables. • A `data.frame`, when `f` is *not* missing (s. below). • An object of class `ExpressionSet`.
`y`	Class labels. Can be one of the following:

- A numeric vector.
- A factor.
- A character if X is an ExpressionSet that specifies the phenotype variable.
- missing, if X is a data.frame and a proper formula f is provided.

WARNING: The class labels will be re-coded to range from 0 to K-1, where K is the total number of different classes in the learning set.

f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.
learnind	An index vector specifying the observations that belong to the learning set. May be missing; in that case, the learning set consists of all observations and predictions are made on the learning set.
models	a logical value indicating whether the model object shall be returned
...	Further arguments to be passed to lda from the package MASS

Value

An object of class cloutput.

Note

Excessive variable selection has usually to performed before ldaCMA can be applied in the p > n setting. Not reducing the number of variables can result in an error message.

Author(s)

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References

McLachlan, G.J. (1992).

Discriminant Analysis and Statistical Pattern Recognition.

Wiley, New York

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
## Not run:
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression from first 10 genes
golubX <- as.matrix(golub[,2:11])
### select learningset
ratio <- 2/3
```

```
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run LDA
ldaresult <- ldaCMA(X=golubX, y=golubY, learnind=learnind)
### show results
show(ldaresult)
ftable(ldaresult)
plot(ldaresult)
### multiclass example:
### load Khan data
data(khan)
### extract class labels
khanY <- khan[,1]
### extract gene expression from first 10 genes
khanX <- as.matrix(khan[,2:11])
### select learningset
set.seed(111)
learnind <- sample(length(khanY), size=floor(ratio*length(khanY)))
### run LDA
ldaresult <- ldaCMA(X=khanX, y=khanY, learnind=learnind)
### show results
show(ldaresult)
ftable(ldaresult)
plot(ldaresult)

## End(Not run)
```

---

ldaCMA-methods *Linear Discriminant Analysis*

Description

Performs a linear discriminant analysis for the following signatures:

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult ldaCMA.

---

learningsets-class *"learningsets"*

Description

An object returned from GenerateLearningsets which is usually passed as arguments to GeneSelection, tune and classification.

Slots

`learnmatrix`: A matrix of dimension `niter` x `ntrain`. Each row contains the indices of those observations representing the learningset for one iteration. If `method` = `CV`, zeros appear due to rounding issues.

`method`: The method used to generate the `learnmatrix`, s.`GenerateLearningsets`

`ntrain`: Number of observations in one learning set.If `method` = `CV`, this number is not attained for all iterations, due to rounding issues.

`iter`: Number of iterations (different learningsets) that are stored in `learnmatrix`.

Methods

- showUse `show(learningsets-object)` for brief information.

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Christoph Bernau <bernau@ibe.med.uni-muenchen.de>

See Also

`GenerateLearningsets`, `GeneSelection`, `tune`, `classification`

---

nnetCMA *Feed-forward Neural Networks*

Description

This method provides access to the function `nnet` in the package of the same name that trains Feed-forward Neural Networks with one hidden layer.
For `S4` method information, see nnetCMA-methods

Usage

```
nnetCMA(X, y, f, learnind, eigengenes = FALSE, models=FALSE,...)
```

Arguments

`X`	Gene expression data. Can be one of the following: • A `matrix`. Rows correspond to observations, columns to variables. • A `data.frame`, when `f` is *not* missing (s. below). • An object of class `ExpressionSet`.
`y`	Class labels. Can be one of the following: • A `numeric` vector. • A `factor`. • A `character` if `X` is an `ExpressionSet` that specifies the phenotype variable. • `missing`, if `X` is a `data.frame` and a proper formula `f` is provided.

WARNING: The class labels will be re-coded to range from `0` to `K-1`, where `K` is the total number of different classes in the learning set.

`f` A two-sided formula, if `X` is a `data.frame`. The left part correspond to class labels, the right to variables.

`learnind` An index vector specifying the observations that belong to the learning set. May be `missing`; in that case, the learning set consists of all observations and predictions are made on the learning set.

`eigengenes` Should the training be performed be in the space of eigengenes obtained from a singular value decomposition of the Gene expression data matrix ? Default is `FALSE`; in this case, variable selection is necessary to reduce the number of weights that have to be optimized.

`models` a logical value indicating whether the model object shall be returned

`...` Further arguments passed to the function `nnet` from the package of the same name.
Important parameters are:

- `"size"`, i.e. the number of units in the hidden layer
- `"decay"` for weight decay.

Value

An object of class `cloutput`.

Note

- Excessive variable selection is usually necessary if `eigengenes = FALSE`
- Different runs of this method on the same dataset not necessarily produce the same results due to the fact that optimization for Feed-Forward Neural Networks is rather difficult and depends on the choice of (normally randomly chosen) starting values for the network weights.

Author(s)

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Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

Christoph Bernau <bernau@ibe.med.uni-muenchen.de>

References

Ripley, B.D. (1996)
Pattern Recognition and Neural Networks.
Cambridge University Press

See Also

`compBoostCMA`, `dldaCMA`, `ElasticNetCMA`, `fdaCMA`, `flexdaCMA`, `gbmCMA`, `knnCMA`, `ldaCMA`, `LassoCMA`, `nnetCMA`, `pknnCMA`, `plrCMA`, `pls_ldaCMA`, `pls_lrCMA`, `pls_rfCMA`, `pnnCMA`, `qdaCMA`, `rfCMA`, `scdaCMA`, `shrinkldaCMA`, `svmCMA`

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression from first 10 genes
golubX <- as.matrix(golub[,2:11])
### select learningset
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run nnet (not tuned)
nnetresult <- nnetCMA(X=golubX, y=golubY, learnind=learnind, size = 3, decay = 0.01)
### show results
show(nnetresult)
ftable(nnetresult)
plot(nnetresult)
### in the space of eigengenes (not tuned)
golubXfull <-  as.matrix(golubX[,-1])
nnetresult <- nnetCMA(X=golubXfull, y=golubY, learnind = learnind, eigengenes = TRUE,
                      size = 3, decay = 0.01)
### show results
show(nnetresult)
ftable(nnetresult)
plot(nnetresult)
```

---

nnetCMA-methods *Feed-Forward Neural Networks*

Description

This method provides access to the function `nnet` in the package of the same name that trains Feed-forward Neural Networks with one hidden layer.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult `nnetCMA`.

obsinfo *Classifiability of observations*

Description

Some observations are harder to classify than others. It is frequently of interest to know which observations are consistenly misclassified; these are candiates for outliers or wrong class labels.

Arguments

object	An object of class evaluation, generated with scheme = "observationwise"
threshold	threshold value of (observation-wise) performance measure, s. evaluation that has to be exceeded in order to speak of consistent misclassification. If measure = "average probability", then values *below* threshold are regarded as consistent misclassification. Note that the default values 1 is not sensible in that case
show	Should the information be printed ? Default is TRUE.

Details

As not all observation must have been classified at least once, observations not classified at all are also shown.

Value

A list with two components

misclassification
: A data.frame containing the indices of consistenly misclassfied observations and the corresponding performance measure.

notclassified
: The indices of those observations not classfied at all, s. details.

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

See Also

evaluation

pknnCMA *Probabilistic Nearest Neighbours*

Description

Nearest neighbour variant that replaces the simple voting scheme by a weighted one (based on euclidean distances). This is also used to compute class probabilities.

For S4 class information, see pknnCMA-methods.

Usage

```
pknnCMA(X, y, f, learnind, beta = 1, k = 1, models=FALSE, ...)
```

Arguments

X	Gene expression data. Can be one of the following: • A matrix. Rows correspond to observations, columns to variables. • A data.frame, when f is *not* missing (s. below). • An object of class ExpressionSet.
y	Class labels. Can be one of the following: • A numeric vector. • A factor. • A character if X is an ExpressionSet that specifies the phenotype variable. • missing, if X is a data.frame and a proper formula f is provided. **WARNING**: The class labels will be re-coded to range from 0 to K-1, where K is the total number of different classes in the learning set.
f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.
learnind	An index vector specifying the observations that belong to the learning set. Must not be missing for this method.
beta	Slope parameter for the logistic function which is used for the computation of class probabilities. The default value (1) need not produce reasonable results and can produce warnings.
k	Number of nearest neighbours to use.
models	a logical value indicating whether the model object shall be returned
...	Currently unused argument.

Details

The algorithm is as follows:

- Determine the k nearest neighbours
- For each class represented among these, compute the average euclidean distance.
- The negative distances are plugged into the logistic function with parameter beta.
- Classify into the class with highest probability.

Value

An object of class cloutput.

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression from first 10 genes
golubX <- as.matrix(golub[,-1])
### select learningset
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run probabilistic k-nearest neighbours
result <- pknnCMA(X=golubX, y=golubY, learnind=learnind, k = 3)
### show results
show(result)
ftable(result)
plot(result)
```

---

pknnCMA-methods *Probabilistic nearest neighbours*

Description

Nearest neighbour variant that replaces the simple voting scheme by a weighted one (based on euclidean distances). This is also used to compute class probabilities.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult pknnCMA.

Planarplot *Visualize Separability of different classes*

Description

Given two variables, the methods trains a classifier (argument `classifier`) based on these two variables and plots the resulting class regions, learning- and test observations in the plane.

Appropriate variables are usually found by `GeneSelection`.

For S4 method information, s. `Planarplot-methods`.

Usage

```
Planarplot(X, y, f, learnind, predind, classifier, gridsize = 100, ...)
```

Arguments

`X`	Gene expression data. Can be one of the following: • A `matrix`. Rows correspond to observations, columns to variables. • A `data.frame`, when `f` is *not* missing (s. below). • An object of class `ExpressionSet`.
`y`	Class labels. Can be one of the following: • A `numeric` vector. • A `factor`. • A `character` if `X` is an `ExpressionSet` that specifies the phenotype variable. • `missing`, if `X` is a `data.frame` and a proper formula `f` is provided.
`f`	A two-sided formula, if `X` is a `data.frame`. The left part correspond to class labels, the right to variables.
`learnind`	An index vector specifying the observations that belong to the learning set. May be `missing`; in that case, the learning set consists of all observations and predictions are made on the learning set.
`predind`	A vector containing *exactly* two indices that denote the two variables used for classification.
`classifier`	Name of function ending with `CMA` indicating the classifier to be used.
`gridsize`	The gridsize used for two-dimensional plotting. For both variables specified in `predind`, an equidistant grid of size `gridsize` is created. The resulting two grids are then combined to obtain `gridsize^2` points in the real plane which are used to draw the class regions. Defaults to 100 which is usually a reasonable choice, but takes some time.
`...`	Further argument passed to `classifier`.

Value

No return.

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>. Idea is from the MLInterfaces package, contributed by Jess Mar, Robert Gentleman and Vince Carey.

See Also

GeneSelection, compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### simple linear discrimination for the golub data:
data(golub)
golubY <- golub[,1]
golubX <- as.matrix(golub[,-1])
golubn <- nrow(golubX)
set.seed(111)
learnind <- sample(golubn, size=floor(2/3*golubn))
Planarplot(X=golubX, y=golubY, learnind=learnind, predind=c(2,4),
           classifier=ldaCMA)
```

Planarplot-methods *Visualize Separability of different classes*

Description

Given two variables, the methods trains a classifier (argument classifier) based on these two variables and plots the resulting class regions, learning- and test observations in the plane.

Appropriate variables are usually found by GeneSelection.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult Planarplot.

plot *Probability plot*

Description

A popular way of visualizing the output of classifier is to plot, separately for each class, the predicted probability of each predicted observations for the respective class. For this purpose, the plot area is divided into K parts, where K is the number of classes. Predicted observations are assigned, according to their true class, to one of those parts. Then, for each part and each predicted observation, the predicted probabilities are plotted, displayed by coloured dots, where each colour corresponds to one class.

Arguments

x	An object of class cloutput whose slot probmatrix does not contain any missing value, i.e. probability estimations are provided by the classifier.
main	A title for the plot (character).

Value

No return.

Note

The plot usually only makes sense if a sufficiently large numbers of observations has been classified. This is usually achieved by running the classifier on several learningsets with the method classification. The output can then be processed via join to obtain an object of class cloutput to which this method can be applied.

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

See Also

cloutput

plot tuningresult *Visualize results of tuning*

Description

After hyperparameter tuning using tune it is useful to see which choice of hyperparameters is suitable and how good the performance is.

Arguments

x	An object of class tuningresult.
iter	Iteration number (learningset) for which tuning results should be displayed.
which	Character vector (maximum length is two) naming the arguments for which tuning results should be display. Default is NULL; if the number of tuned hyperparameter is less or equal than two, then the results for these hyperparameters will be plotted. If this number is two, then a contour plot will be made, otherwise a simple line segment plot. If the number of tuned hyperparameters exceeds two, then which may not be NULL.
...	Further graphical options passed either to plot or contour.

Value

no return.

Note

Frequently, several hyperparameter (combinations) perform "best", s. also the remark in best.

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

See Also

tune, tuningresult

plrCMA *L2 penalized logistic regression*

Description

High dimensional logistic regression combined with an L2-type (Ridge-)penalty. Multiclass case is also possible. For S4 method information, see plrCMA-methods

Usage

```
plrCMA(X, y, f, learnind, lambda = 0.01, scale = TRUE, models=FALSE,...)
```

Arguments

X	Gene expression data. Can be one of the following: • A matrix. Rows correspond to observations, columns to variables. • A data.frame, when f is *not* missing (s. below). • An object of class ExpressionSet.
y	Class labels. Can be one of the following: • A numeric vector. • A factor. • A character if X is an ExpressionSet that specifies the phenotype variable. • missing, if X is a data.frame and a proper formula f is provided. **WARNING**: The class labels will be re-coded to range from 0 to K-1, where K is the total number of different classes in the learning set.
f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.
learnind	An index vector specifying the observations that belong to the learning set. May be missing; in that case, the learning set consists of all observations and predictions are made on the learning set.
lambda	Parameter governing the amount of penalization. This hyperparameter should be tuned.
scale	Scale the predictors as specified by X to have unit variance and zero mean.
models	a logical value indicating whether the model object shall be returned
...	Currently unused argument.

Value

An object of class cloutput.

Author(s)

Special thanks go to

Ji Zhu (University of Ann Arbor, Michigan)

Trevor Hastie (Stanford University)

who provided the basic code that was then adapted by

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>.

References

Zhu, J., Hastie, T. (2004). Classification of gene microarrays by penalized logistic regression. *Biostatistics 5:427-443*.

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression from first 10 genes
golubX <- as.matrix(golub[,-1])
### select learningset
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run penalized logistic regression (no tuning)
plrresult <- plrCMA(X=golubX, y=golubY, learnind=learnind)
### show results
show(plrresult)
ftable(plrresult)
plot(plrresult)
### multiclass example:
### load Khan data
data(khan)
### extract class labels
khanY <- khan[,1]
### extract gene expression from first 10 genes
khanX <- as.matrix(khan[,-1])
### select learningset
set.seed(111)
learnind <- sample(length(khanY), size=floor(ratio*length(khanY)))
### run penalized logistic regression (no tuning)
plrresult <- plrCMA(X=khanX, y=khanY, learnind=learnind)
### show results
show(plrresult)
ftable(plrresult)
plot(plrresult)
```

---

plrCMA-methods *L2 penalized logistic regression*

Description

High dimensional logistic regression combined with an L2-type (Ridge-)penalty. Multiclass case is also possible.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult `plrCMA`.

---

pls_ldaCMA *Partial Least Squares combined with Linear Discriminant Analysis*

Description

This method constructs a classifier that extracts Partial Least Squares components that are plugged into Linear Discriminant Analysis. The Partial Least Squares components are computed by the package `plsgenomics`.

For `S4` method information, see `pls_ldaCMA-methods`.

Usage

```
pls_ldaCMA(X, y, f, learnind, comp = 2, plot = FALSE,models=FALSE)
```

Arguments

`X`	Gene expression data. Can be one of the following: • A `matrix`. Rows correspond to observations, columns to variables. • A `data.frame`, when `f` is *not* missing (s. below). • An object of class `ExpressionSet`.
`y`	Class labels. Can be one of the following: • A `numeric` vector. • A `factor`. • A `character` if `X` is an `ExpressionSet` that specifies the phenotype variable. • `missing`, if `X` is a `data.frame` and a proper formula `f` is provided. **WARNING**: The class labels will be re-coded to range from `0` to `K-1`, where `K` is the total number of different classes in the learning set.
`f`	A two-sided formula, if `X` is a `data.frame`. The left part correspond to class labels, the right to variables.
`learnind`	An index vector specifying the observations that belong to the learning set. May be `missing`; in that case, the learning set consists of all observations and predictions are made on the learning set.
`comp`	Number of Partial Least Squares components to extract. Default is 2 which can be suboptimal, depending on the particular dataset. Can be optimized using `tune`.
`plot`	If `comp <= 2`, should the classification space of the Partial Least Squares components be plotted ? Default is `FALSE`.
`models`	a logical value indicating whether the model object shall be returned

Value

An object of class cloutput.

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Nguyen, D., Rocke, D. M., (2002).

Tumor classifcation by partial least squares using microarray gene expression data.

Bioinformatics 18, 39-50

Boulesteix, A.L., Strimmer, K. (2007).

Partial least squares: a versatile tool for the analysis of high-dimensional genomic data.

Briefings in Bioinformatics 7:32-44.

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
## Not run:
### load Khan data
data(khan)
### extract class labels
khanY <- khan[,1]
### extract gene expression
khanX <- as.matrix(khan[,-1])
### select learningset
set.seed(111)
learnind <- sample(length(khanY), size=floor(2/3*length(khanY)))
### run Shrunken Centroids classfier, without tuning
plsresult <- pls_ldaCMA(X=khanX, y=khanY, learnind=learnind, comp = 4)
### show results
show(plsresult)
ftable(plsresult)
plot(plsresult)
## End(Not run)
```

---

pls_ldaCMA-methods *Partial Least Squares combined with Linear Discriminant Analysis*

Description

-This method constructs a classifier that extracts Partial Least Squares components that are plugged into Linear Discriminant Analysis. The Partial Least Squares components are computed by the package plsgenomics.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult `pls_ldaCMA`.

`pls_lrCMA` *Partial Least Squares followed by logistic regression*

Description

This method constructs a classifier that extracts Partial Least Squares components that form the the covariates in a binary logistic regression model. The Partial Least Squares components are computed by the package `plsgenomics`.

For `S4` method information, see `pls_lrCMA-methods`.

Usage

```
pls_lrCMA(X, y, f, learnind, comp = 2, lambda = 1e-4, plot = FALSE,models=FALSE)
```

Arguments

`X`	Gene expression data. Can be one of the following: • A `matrix`. Rows correspond to observations, columns to variables. • A `data.frame`, when `f` is *not* missing (s. below). • An object of class `ExpressionSet`.
`y`	Class labels. Can be one of the following: • A `numeric` vector. • A `factor`. • A `character` if `X` is an `ExpressionSet` that specifies the phenotype variable. • `missing`, if `X` is a `data.frame` and a proper formula `f` is provided. **WARNING**: The class labels will be re-coded to range from `0` to `K-1`, where `K` is the total number of different classes in the learning set.
`f`	A two-sided formula, if `X` is a `data.frame`. The left part correspond to class labels, the right to variables.
`learnind`	An index vector specifying the observations that belong to the learning set. May be `missing`; in that case, the learning set consists of all observations and predictions are made on the learning set.
`comp`	Number of Partial Least Squares components to extract. Default is 2 which can be suboptimal, depending on the particular dataset. Can be optimized using `tune`.
`lambda`	Parameter controlling the amount of L2 penalization for logistic regression, usually taken to be a small value in order to stabilize estimation in the case of separable data.
`plot`	If `comp <= 2`, should the classification space of the Partial Least Squares components be plotted ? Default is `FALSE`.
`models`	a logical value indicating whether the model object shall be returned

Value

An object of class cloutput.

Note

Up to now, only the two-class case is supported.

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Boulesteix, A.L., Strimmer, K. (2007).

Partial least squares: a versatile tool for the analysis of high-dimensional genomic data.

Briefings in Bioinformatics 7:32-44.

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression
golubX <- as.matrix(golub[,-1])
### select learningset
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run PLS, combined with logistic regression
result <- pls_lrCMA(X=golubX, y=golubY, learnind=learnind)
### show results
show(result)
ftable(result)
plot(result)
```

---

pls_lrCMA-methods *Partial Least Squares followed by logistic regression*

Description

This method constructs a classifier that extracts Partial Least Squares components that form the the covariates in a binary logistic regression model. The Partial Least Squares components are computed by the package plsgenomics.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult `pls_lrCMA`

`pls_rfCMA` *Partial Least Squares followed by random forests*

Description

This method constructs a classifier that extracts Partial Least Squares components used to generate Random Forests, s. `rfCMA`.

For `S4` method information, see `pls_rfCMA-methods`.

Usage

```
pls_rfCMA(X, y, f, learnind, comp = 2 * nlevels(as.factor(y)), seed = 111,models=FALSE, ...)
```

Arguments

`X`	Gene expression data. Can be one of the following: • A `matrix`. Rows correspond to observations, columns to variables. • A `data.frame`, when `f` is *not* missing (s. below). • An object of class `ExpressionSet`.
`y`	Class labels. Can be one of the following: • A `numeric` vector. • A `factor`. • A `character` if `X` is an `ExpressionSet` that specifies the phenotype variable. • `missing`, if `X` is a `data.frame` and a proper formula `f` is provided. **WARNING**: The class labels will be re-coded to range from `0` to `K-1`, where `K` is the total number of different classes in the learning set.
`f`	A two-sided formula, if `X` is a `data.frame`. The left part correspond to class labels, the right to variables.
`learnind`	An index vector specifying the observations that belong to the learning set. May be `missing`; in that case, the learning set consists of all observations and predictions are made on the learning set.
`comp`	Number of Partial Least Squares components to extract. Default ist two times the number of different classes.
`seed`	Fix Random number generator seed to `seed`. This is useful to guarantee reproducibility of the results, due to the random component in the random Forest.
`models`	a logical value indicating whether the model object shall be returned
`...`	Further arguments to be passed to `randomForests` from the package of the same name.

Value

An object of class cloutput.

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Boulesteix, A.L., Strimmer, K. (2007).

Partial least squares: a versatile tool for the analysis of high-dimensional genomic data.

Briefings in Bioinformatics 7:32-44.

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression
golubX <- as.matrix(golub[,-1])
### select learningset
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run PLS, combined with Random Forest
#result <- pls_rfCMA(X=golubX, y=golubY, learnind=learnind)
### show results
#show(result)
#ftable(result)
#plot(result)
```

---

pls_rfCMA-methods *Partial Least Squares followed by random forests*

Description

This method constructs a classifier that extracts Partial Least Squares components used to generate Random Forests, s. rfCMA. The Partial Least Squares components are computed by the package plsgenomics.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult `pls_rfCMA`.

`pnnCMA` *Probabilistic Neural Networks*

Description

Probabilistic Neural Networks is the term Specht (1990) used for a Gaussian kernel estimator for the conditional class densities.

For `S4` method information, see pnnCMA-methods.

Usage

```
pnnCMA(X, y, f, learnind, sigma = 1,models=FALSE)
```

Arguments

`X`	Gene expression data. Can be one of the following: • A `matrix`. Rows correspond to observations, columns to variables. • A `data.frame`, when `f` is *not* missing (s. below). • An object of class `ExpressionSet`. Each variable (gene) will be scaled for unit variance and zero mean.
`y`	Class labels. Can be one of the following: • A `numeric` vector. • A `factor`. • A `character` if `X` is an `ExpressionSet` that specifies the phenotype variable. • `missing`, if `X` is a `data.frame` and a proper formula `f` is provided. **WARNING**: The class labels will be re-coded to range from `0` to `K-1`, where `K` is the total number of different classes in the learning set.
`f`	A two-sided formula, if `X` is a `data.frame`. The left part correspond to class labels, the right to variables.
`learnind`	An index vector specifying the observations that belong to the learning set. For this method, this must *not* be `missing`.
`sigma`	Standard deviation of the Gaussian Kernel used. This hyperparameter should be tuned, s. `tune`. The default is `1`, but this generally does not lead to good results. Actually, this method reacts very sensitively to the value of sigma. Take care if warnings appear related to the particular choice.
`models`	a logical value indicating whether the model object shall be returned

Value

An object of class cloutput.

Note

There is actually no strong relation of this method to Feed-Forward Neural Networks, s. nnetCMA.

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Specht, D.F. (1990).

Probabilistic Neural Networks. *Neural Networks, 3, 109-118*.

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression from first 10 genes
golubX <- as.matrix(golub[,2:11])
### select learningset
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run PNN
pnnresult <- pnnCMA(X=golubX, y=golubY, learnind=learnind, sigma = 3)
### show results
show(pnnresult)
ftable(pnnresult)
plot(pnnresult)
```

---

pnnCMA-methods *Probabilistic Neural Networks*

Description

Probabilistic Neural Networks is the term Specht (1990) used for a Gaussian kernel estimator for the conditional class densities.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For references, further argument and output information, consult pnnCMA.

---

prediction *General method for predicting classes of new observations*

Description

This method constructs the given classifier using the specified training data, gene selection and tuning results.. Subsequently, class labels are predicted for new observations.
For S4 method information, s. classification-methods.

Usage

```
prediction(X.tr,y.tr,X.new,f,classifier,genesel,models=F,nbgene,tuneres,...)
```

Arguments

X.tr	Training gene expression data. Can be one of the following: • A matrix. Rows correspond to observations, columns to variables. • A data.frame, when f is *not* missing (s. below). • An object of class ExpressionSet.
X.new	gene expression data. Can be one of the following: • A matrix. Rows correspond to observations, columns to variables. • A data.frame, when f is *not* missing (s. below). • An object of class ExpressionSet.
y.tr	Class labels of training observation. Can be one of the following: • A numeric vector. • A factor. • A character if X is an ExpressionSet that specifies the phenotype variable. • missing, if X is a data.frame and a proper formula f is provided. **WARNING**: The class labels will be re-coded for classifier construction to range from 0 to K-1, where K is the total number of different classes in the learning set.
f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.
genesel	Optional (but usually recommended) object of class genesel containing variable importance information for the argument learningsets. In this case the object contains a single variable selection. Appropriate genesel-objects can be obtained using the function genesel without learningset and setting X=X.tr and y=y.tr (i.e. corresponding to the training data of this function).

nbgene — Number of best genes to be kept for classification, based on either genesel or the call to GeneSelection using geneselllist. In the case that both are missing, this argument is not necessary. **note**:

- If the gene selection method has been one of "lasso", "elasticnet", "boosting", nbgene will be reset to min(s, nbgene) where s is the number of nonzero coefficients.
- if the gene selection scheme has been "one-vs-all", "pairwise" for the multiclass case, there exist several rankings. The top nbgene will be kept of *each* of them, so the number of effective used genes will sometimes be much larger.

classifier — Name of function ending with CMA indicating the classifier to be used.

tuneres — Analogous to the argument genesel - object of class tuningresult containing information about the best hyperparameter choice for the argument learningsets. Appropriate tuning-objects can be obtained using the function tune without learningsets and setting parameters X=X.tr, y=y.tr and genesel=genesel (i.e. using the same training data and gene selection as in this function)

models — a logical value indicating whether the model object shall be returned

... — Further arguments passed to the function classifier.

Details

This function builds the specified classifier and predicts the class labels of new observations. Hence, its usage differs from those of most other prediction functions in R.

Value

A object of class predoutput-class; Predicted classes can be seen by show(predoutput)

Author(s)

Christoph Bernau <bernau@ibe.med.uni-muenchen.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

See Also

GeneSelection, tune, evaluation, compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMAclassification

Examples

```
### a simple k-nearest neighbour example
### datasets
## Not run: plot(x)
data(golub)
golubY <- golub[,1]
golubX <- as.matrix(golub[,-1])
```

```
###Splitting data into training and test set
X.tr<-golubX[1:30]
X.new<-golubX[31:39]
y.tr<-golubY[1:30]
### 1. GeneSelection
selttest <- GeneSelection(X=X.tr, y=y.tr, method = "t.test")
### 2. tuning
tunek <- tune(X.tr, y.tr, genesel = selttest, nbgene = 20, classifier = knnCMA)
### 3. classification
pred <- prediction(X.tr=X.tr,y.tr=y.tr,X.new=X.new, genesel = selttest,
                       tuneres = tunek, nbgene = 20, classifier = knnCMA)
### show and analyze results:
show(pred)


## End(Not run)
```

`prediction-methods` *General method for predicting class lables of new observations*

Description

Perform prediction signatures:

Methods

X.tr = "matrix", X.new="matrix", y.tr='any',f = "missing" signature 1

X.tr = "data.frame", X.new="data.frame", y.tr = "missing", f = "formula" signature 2

X.tr = "ExpressionSet",X.new = "ExpressionSet", y.tr = "character", f = "missing" signature 3

For further argument and output information, consult `classification`.

`predoutput-class` *"predoutput"*

Description

Object returned by the function `prediction`

Slots

`Xnew`**:** Gene Expression matrix of new observations

`yhat`**:** Predicted class labels for the new data.

`model`**:** List containing the constructed classifier.

Methods

show Returns predicted class labels for the new data.

Author(s)

Christoph Bernau <bernau@ibe.med.uni-muenchen.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

---

qdaCMA *Quadratic Discriminant Analysis*

Description

Performs a quadratic discriminant analysis under the assumption of a multivariate normal distribution in each classes without restriction concerning the covariance matrices. The function qda from the package MASS is called for computation.

For S4 method information, see qdaCMA-methods.

Usage

```
qdaCMA(X, y, f, learnind,models=FALSE, ...)
```

Arguments

X	Gene expression data. Can be one of the following: • A matrix. Rows correspond to observations, columns to variables. • A data.frame, when f is *not* missing (s. below). • An object of class ExpressionSet.
y	Class labels. Can be one of the following: • A numeric vector. • A factor. • A character if X is an ExpressionSet that specifies the phenotype variable. • missing, if X is a data.frame and a proper formula f is provided. **WARNING**: The class labels will be re-coded to range from 0 to K-1, where K is the total number of different classes in the learning set.
f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.
learnind	An index vector specifying the observations that belong to the learning set. May be missing; in that case, the learning set consists of all observations and predictions are made on the learning set.
models	a logical value indicating whether the model object shall be returned
...	Further arguments to be passed to qda from the package MASS

Value

An object of class cloutput.

Note

Excessive variable selection has usually to performed before qdaCMA can be applied in the p > n setting. Not reducing the number of variables can result in an error message.

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

McLachlan, G.J. (1992).

Discriminant Analysis and Statistical Pattern Recognition.

Wiley, New York

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, rfCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression from first 3 genes
golubX <- as.matrix(golub[,2:4])
### select learningset
ratio <- 2/3
set.seed(112)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run QDA
qdaresult <- qdaCMA(X=golubX, y=golubY, learnind=learnind)
### show results
show(qdaresult)
ftable(qdaresult)
plot(qdaresult)
### multiclass example:
### load Khan data
data(khan)
### extract class labels
khanY <- khan[,1]
### extract gene expression from first 4 genes
khanX <- as.matrix(khan[,2:5])
### select learningset
set.seed(111)
learnind <- sample(length(khanY), size=floor(ratio*length(khanY)))
### run QDA
```

```
qdaresult <- qdaCMA(X=khanX, y=khanY, learnind=learnind)
### show results
show(qdaresult)
ftable(qdaresult)
plot(qdaresult)
```

---

qdaCMA-methods *Quadratic Discriminant Analysis*

Description

Performs a quadratic discriminant analysis under the assumption of a multivariate normal distribution in each classes without restriction concerning the covariance matrices. The function qda from the package MASS is called for computation.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult qdaCMA.

---

rfCMA *Classification based on Random Forests*

Description

Random Forests were proposed by Breiman (2001) and are implemented in the package randomForest.

In this package, they can as well be used to rank variables according to their importance, s. GeneSelection.

For S4 method information, see rfCMA-methods

Usage

```
rfCMA(X, y, f, learnind, varimp = TRUE, seed = 111, models=FALSE,type=1,scale=FALSE,importance=TRUE
```

Arguments

X	Gene expression data. Can be one of the following: • A matrix. Rows correspond to observations, columns to variables. • A data.frame, when f is *not* missing (s. below). • An object of class ExpressionSet.
y	Class labels. Can be one of the following: • A numeric vector. • A factor. • A character if X is an ExpressionSet that specifies the phenotype variable.

- missing, if X is a data.frame and a proper formula f is provided.

WARNING: The class labels will be re-coded to range from 0 to K-1, where K is the total number of different classes in the learning set.

f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.
learnind	An index vector specifying the observations that belong to the learning set. May be missing; in that case, the learning set consists of all observations and predictions are made on the learning set.
varimp	Should additional information for variable selection be provided ? Defaults to TRUE.
seed	Fix Random number generator seed to seed. This is useful to guarantee reproducibility of the results.
models	a logical value indicating whether the model object shall be returned
type	Parameter passed to function importance. Either 1 or 2, specifying the type of importance measure (1=mean decrease in accuracy, 2=mean decrease in node impurity).
scale	Parameter passed to function importance. For permutation based measures, should the measures be divided by their standard errors?
importance	Parameter passed to function randomForest.Should importance of predictors be assessed by permutation?
...	Further arguments to be passed to randomForest from the package of the same name.

Value

If varimp, then an object of class clvarseloutput is returned, otherwise an object of class cloutput

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Breiman, L. (2001)

Random Forest.

Machine Learning, 45:5-32.

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, scdaCMA, shrinkldaCMA, svmCMA

Examples

```
 ### load Khan data
data(khan)
### extract class labels
khanY <- khan[,1]
### extract gene expression
khanX <- as.matrix(khan[,-1])
### select learningset
set.seed(111)
learnind <- sample(length(khanY), size=floor(2/3*length(khanY)))
### run random Forest
#rfresult <- rfCMA(X=khanX, y=khanY, learnind=learnind, varimp = FALSE)
### show results
#show(rfresult)
#ftable(rfresult)
#plot(rfresult)
```

---

rfCMA-methods *Classification based on Random Forests*

Description

Random Forests were proposed by Breiman (2001) and are implemented in the package randomForest.

In this package, they can as well be used to rank variables according to their importance, s. GeneSelection.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For references, further argument and output information, consult rfCMA

---

roc *Receiver Operator Characteristic*

Description

The empirical Receiver Operator Characteristic (ROC) is widely used for the evaluation of diagnostic tests, but also for the evaluation of classfiers. In this implementation, it can only be used for the binary classification case. The input are a numeric vector of class probabilities (which play the role of a test result) and the true class labels. Note that misclassifcation performance can (partly widely) differ from the Area under the ROC (AUC). This is due to the fact that misclassifcation rates are always computed for the threshold 'probability = 0.5'.

Arguments

object	An object of cloutput.
plot	Should the ROC curve be plotted ? Default is TRUE.
...	Argument to specifiy further graphical options.

Value

The empirical area under the curve (AUC).

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

See Also

evaluation

---

scdaCMA *Shrunken Centroids Discriminant Analysis*

Description

The nearest shrunken centroid classification algorithm is detailly described in Tibshirani et al. (2002).

It is widely known under the name PAM (prediction analysis for microarrays), which can also be found in the package pamr.

For S4 method information, see scdaCMA-methods.

Usage

```
scdaCMA(X, y, f, learnind, delta = 0.5, models=FALSE,...)
```

Arguments

X	Gene expression data. Can be one of the following: • A matrix. Rows correspond to observations, columns to variables. • A data.frame, when f is *not* missing (s. below). • An object of class ExpressionSet.
y	Class labels. Can be one of the following: • A numeric vector. • A factor. • A character if X is an ExpressionSet that specifies the phenotype variable. • missing, if X is a data.frame and a proper formula f is provided. **WARNING**: The class labels will be re-coded to range from 0 to K-1, where K is the total number of different classes in the learning set.
f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.

learnind	An index vector specifying the observations that belong to the learning set. May be missing; in that case, the learning set consists of all observations and predictions are made on the learning set.
delta	The shrinkage intensity for the class centroids - a hyperparameter that must be tuned. The default 0.5 not necessarily produces good results.
models	a logical value indicating whether the model object shall be returned
...	Currently unused argument.

Value

An object of class cloutput.

Note

The results can differ from those obtained by using the package pamr.

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Tibshirani, R., Hastie, T., Narasimhan, B., and Chu, G., (2003).

Class prediction by nearest shrunken centroids with applications to DNA microarrays.

Statistical Science, 18, 104-117

See Also

compBoostCMA, dldaCMA, ElasticNetCMA, fdaCMA, flexdaCMA, gbmCMA, knnCMA, ldaCMA, LassoCMA, nnetCMA, pknnCMA, plrCMA, pls_ldaCMA, pls_lrCMA, pls_rfCMA, pnnCMA, qdaCMA, rfCMA, shrinkldaCMA, svmCMA

Examples

```
### load Khan data
data(khan)
### extract class labels
khanY <- khan[,1]
### extract gene expression
khanX <- as.matrix(khan[,-1])
### select learningset
set.seed(111)
learnind <- sample(length(khanY), size=floor(2/3*length(khanY)))
### run Shrunken Centroids classfier, without tuning
scdaresult <- scdaCMA(X=khanX, y=khanY, learnind=learnind)
### show results
show(scdaresult)
ftable(scdaresult)
plot(scdaresult)
```

scdaCMA-methods *Shrunken Centroids Discriminant Analysis*

Description

The nearest shrunken centroid classification algorithm is detailly described in Tibshirani et al. (2002).

It is widely known under the name PAM (prediction analysis for microarrays), which can also be found in the package `pamr`.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For references, further argument and output information, consult `scdaCMA`.

shrinkldaCMA *Shrinkage linear discriminant analysis*

Description

Linear Discriminant Analysis combined with the James-Stein-Shrinkage approach of Schaefer and Strimmer (2005) for the covariance matrix.

Currently still an experimental version.

For `S4` method information, see shrinkldaCMA-methods

Usage

```
shrinkldaCMA(X, y, f, learnind, models=FALSE, ...)
```

Arguments

`X`	Gene expression data. Can be one of the following: • A `matrix`. Rows correspond to observations, columns to variables. • A `data.frame`, when `f` is *not* missing (s. below). • An object of class `ExpressionSet`.
`y`	Class labels. Can be one of the following: • A `numeric` vector. • A `factor`. • A `character` if `X` is an `ExpressionSet` that specifies the phenotype variable. • `missing`, if `X` is a `data.frame` and a proper formula `f` is provided.

	WARNING: The class labels will be re-coded to range from `0` to `K-1`, where `K` is the total number of different classes in the learning set.
`f`	A two-sided formula, if `X` is a `data.frame`. The left part correspond to class labels, the right to variables.
`learnind`	An index vector specifying the observations that belong to the learning set. May be `missing`; in that case, the learning set consists of all observations and predictions are made on the learning set.
`models`	a logical value indicating whether the model object shall be returned
`...`	Further arguments to be passed to `cov.shrink` from the package `corpcor`

Value

An object of class `cloutput`.

Note

This is still an experimental version.

Covariance shrinkage is performed by calling functions from the package `corpcor`.

Variable selection is *not* necessary.

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

References

Schaefer, J., Strimmer, K. (2005).

A shrinkage approach to large-scale covariance estimation and implications for functional genomics.

Statististical Applications in Genetics and Molecular Biology, 4:32.

See Also

`compBoostCMA`, `dldaCMA`, `ElasticNetCMA`, `fdaCMA`, `flexdaCMA`, `gbmCMA`, `knnCMA`, `ldaCMA`, `LassoCMA`, `nnetCMA`, `pknnCMA`, `plrCMA`, `pls_ldaCMA`, `pls_lrCMA`, `pls_rfCMA`, `pnnCMA`, `qdaCMA`, `rfCMA`, `scdaCMA`, `svmCMA`.

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression
golubX <- as.matrix(golub[,-1])
### select learningset
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run  shrinkage-LDA
result <- shrinkldaCMA(X=golubX, y=golubY, learnind=learnind)
```

```
### show results
show(result)
ftable(result)
plot(result)
```

---

shrinkldaCMA-methods *Shrinkage linear discriminant analysis*

Description

Linear Discriminant Analysis combined with the James-Stein-Shrinkage approach of Schaefer and Strimmer (2005) for the covariance matrix.

Currently still an experimental version. For S4 method information, see shrinkldaCMA-methods

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult shrinkldaCMA.

---

summary *Summarize classifier evaluation*

Description

This method principally does nothing more than applying the pre-implemented summary() function to the slot score of an object of class evaloutput. One then obtains the usual five-point-summary, consisting of minimum and maximum, lower and upper quartile and the median. Additionally, the mean is also shown.

Arguments

object	An object of class evaloutput.
...	Further arguments passed to the pre-implemented summary function.

Value

No return.

Note

That the results normally differ for different evaluation schemes ("iterationwise" or "observationwise").

Author(s)

Martin Slawski <ms@cs.uni-sb.de>

Anne-Laure Boulesteix <boulesteix@ibe.med.uni-muenchen.de>

See Also

evaluation, compare, obsinfo.

---

svmCMA *Support Vector Machine*

Description

Calls the function svm from the package e1071 that provides an interface to the award-winning LIBSVM routines. For S4 method information, see svmCMA-methods

Usage

```
svmCMA(X, y, f, learnind, probability, models=FALSE,seed=341,...)
```

Arguments

X	Gene expression data. Can be one of the following: • A matrix. Rows correspond to observations, columns to variables. • A data.frame, when f is *not* missing (s. below). • An object of class ExpressionSet.
y	Class labels. Can be one of the following: • A numeric vector. • A factor. • A character if X is an ExpressionSet that specifies the phenotype variable. • missing, if X is a data.frame and a proper formula f is provided. **WARNING**: The class labels will be re-coded to range from 0 to K-1, where K is the total number of different classes in the learning set.
f	A two-sided formula, if X is a data.frame. The left part correspond to class labels, the right to variables.
learnind	An index vector specifying the observations that belong to the learning set. May be missing; in that case, the learning set consists of all observations and predictions are made on the learning set.
probability	logical indicating whether the model should allow for probability predictions.
seed	Fix random number generator for reproducibility.
models	a logical value indicating whether the model object shall be returned
...	Further arguments to be passed to svm from the package e1071

Value

An object of class cloutput.

Note

Contrary to the default settings in `e1071:::svm`, the used kernel is a linear kernel which has turned to be out a better default setting in the small sample, large number of predictors - situation, because additional nonlinearity is mostly not necessary there. It additionally avoids the tuning of a further kernel parameter `gamma`, s. help of the package `e1071` for details.
Nevertheless, hyperparameter tuning concerning the parameter `cost` must usually be performed to obtain reasonale results, s. `tune`.

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References

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A training algorithm for optimal margin classifiers.
Proceedings of the fifth annual workshop on Computational learning theory, pages 144-152, ACM Press.

Chang, Chih-Chung and Lin, Chih-Jen : LIBSVM: a library for Support Vector Machines http://www.csie.ntu.edu.tw/~cjlin/libsvm

Schoelkopf, B., Smola, A.J. (2002)
Learning with kernels. *MIT Press, Cambridge, MA*.

See Also

`compBoostCMA`, `dldaCMA`, `ElasticNetCMA`, `fdaCMA`, `flexdaCMA`, `gbmCMA`, `knnCMA`, `ldaCMA`, `LassoCMA`, `nnetCMA`, `pknnCMA`, `plrCMA`, `pls_ldaCMA`, `pls_lrCMA`, `pls_rfCMA`, `pnnCMA`, `qdaCMA`, `rfCMA`, `scdaCMA`, `shrinkldaCMA`

Examples

```
### load Golub AML/ALL data
data(golub)
### extract class labels
golubY <- golub[,1]
### extract gene expression
golubX <- as.matrix(golub[,-1])
### select learningset
ratio <- 2/3
set.seed(111)
learnind <- sample(length(golubY), size=floor(ratio*length(golubY)))
### run _untuned_linear SVM
svmresult <- svmCMA(X=golubX, y=golubY, learnind=learnind,probability=TRUE)
### show results
show(svmresult)
ftable(svmresult)
plot(svmresult)
```

svmCMA-methods *Support Vector Machine*

Description

Calls the function svm from the package e1071 that provides an interface to the award-winning LIBSVM routines.

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult svmCMA.

toplist *Display 'top' variables*

Description

This is a convenient method to get quick access to the most important variables, based on the result of call to GeneSelection.

Usage

```
toplist(object, k = 10, iter = 1, show = TRUE, ...)
```

Arguments

object	An object of genesel.
k	Number of top genes for which information should be displayed. Defaults to 10.
iter	teration number (learningset) for which tuning results should be displayed.
show	Should the results be printed ? Default is TRUE.
...	Currently unused argument.

Value

The type of output depends on the gene selection scheme. For the multiclass case, if gene selection has been run with the "pairwise" or "one-vs-all" scheme, then the output will be a list of data.frames, each containing the gene indices plus variable importance for the top k genes. The list elements are named according to the binary scenarios (e.g., 1 vs. 3). Otherwise, a single data.frame is returned.

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References

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

See Also

genesel, GeneSelection, plot,genesel-method

---

tune *Hyperparameter tuning for classifiers*

Description

Most classifiers implemented in this package depend on one or even several hyperparameters (s. details) that should be optimized to obtain good (and comparable !) results. As tuning scheme, we propose three fold Cross-Validation on each `learningset` (for fixed selected variables). Note that `learningsets` usually do not contain the complete dataset, so tuning involves a second level of splitting the dataset. Increasing the number of folds leads to larger datasets (and possibly to higher accuracy), but also to higher computing times.
For S4 method information, s. `link{tune-methods}`

Usage

```
tune(X, y, f, learningsets, genesel, genesellist = list(), nbgene, classifier, fold = 3, strat = FALS
```

Arguments

`X`	Gene expression data. Can be one of the following: • A `matrix`. Rows correspond to observations, columns to variables. • A `data.frame`, when `f` is *not* missing (s. below). • An object of class `ExpressionSet`.
`y`	Class labels. Can be one of the following: • A `numeric` vector. • A `factor`. • A `character` if `X` is an `ExpressionSet` that specifies the phenotype variable. • `missing`, if `X` is a `data.frame` and a proper formula `f` is provided.
`f`	A two-sided formula, if `X` is a `data.frame`. The left part correspond to class labels, the right to variables.
`learningsets`	An object of class `learningsets`. May be missing, then the complete datasets is used as learning set.
`genesel`	Optional (but usually recommended) object of class `genesel` containing variable importance information for the argument `learningsets`
`genesellist`	In the case that the argument `genesel` is missing, this is an argument list passed to `GeneSelection`. If both `genesel` and `genesellist` are missing, no variable selection is performed.

nbgene	Number of best genes to be kept for classification, based on either genesel or the call to GeneSelection using geneselllist. In the case that both are missing, this argument is not necessary. **note**: • If the gene selection method has been one of "lasso", "elasticnet", "boosting", nbgene will be reset to min(s, nbgene) where s is the number of nonzero coefficients. • if the gene selection scheme has been "one-vs-all", "pairwise" for the multiclass case, there exist several rankings. The top nbgene will be kept of *each* of them, so the number of effective used genes will sometimes be much larger.
classifier	Name of function ending with CMA indicating the classifier to be used.
fold	The number of cross-validation folds used within each learningset. Default is 3. Increasing fold will lead to higher computing times.
strat	Should stratified cross-validation according to the class proportions in the complete dataset be used ? Default is FALSE.
grids	A named list. The names correspond to the arguments to be tuned, e.g. k (the number of nearest neighbours) for knnCMA, or cost for svmCMA. Each element is a numeric vector defining the grid of candidate values. Of course, several hyperparameters can be tuned simultaneously (though requiring much time). By default, grids is an empty list. In that case, a pre-defined list will be used, s. details.
trace	Should progress be traced ? Default is TRUE.
...	Further arguments to be passed to classifier, of course not one of the arguments to be tuned (!).

Details

The following default settings are used, if the arguments grids is an empty list:

```
gbmCMA n.trees = c(50, 100, 200, 500, 1000)
compBoostCMA mstop = c(50, 100, 200, 500, 1000)
LassoCMA norm.fraction = seq(from=0.1, to=0.9, length=9)
ElasticNetCMA norm.fraction = seq(from=0.1, to=0.9, length=5), alpha = 2^{-(5:1)}
plrCMA lambda = 2^{-4:4}
pls_ldaCMA comp = 1:10
pls_lrCMA comp = 1:10
pls_rfCMA comp = 1:10
rfCMA mtry = ceiling(c(0.1, 0.25, 0.5, 1, 2)*sqrt(ncol(X))), nodesize = c(1,2,3)
knnCMA k=1:10
pknnCMA k = 1:10
scdaCMA delta = c(0.1, 0.25, 0.5, 1, 2, 5)
pnnCMA sigma = c(2^{-2:2}),
nnetCMA size = 1:5, decay = c(0, 2^{-(4:1)})
svmCMA, kernel = "linear" cost = c(0.1, 1, 5, 10, 50, 100, 500)
svmCMA, kernel = "radial" cost = c(0.1, 1, 5, 10, 50, 100, 500), gamma = 2^{-2:2}
svmCMA, kernel = "polynomial" cost = c(0.1, 1, 5, 10, 50, 100, 500), degree = 2:4
```

Value

An object of class tuningresult

Note

The computation time can be enormously high. Note that for each different learningset, the classifier must be trained fold times number of possible different hyperparameter combinations times. E.g. if the number of the learningsets is fifty, fold = 3 and two hyperparameters (each with 5 candidate values) are tuned, 50x3x25=3750 training iterations are necessary !

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References

Slawski, M. Daumer, M. Boulesteix, A.-L. (2008) CMA - A comprehensive Bioconductor package for supervised classification with high dimensional data. *BMC Bioinformatics 9: 439*

See Also

tuningresult, GeneSelection, classification

Examples

```
## Not run:
### simple example for a one-dimensional grid, using compBoostCMA.
### dataset
data(golub)
golubY <- golub[,1]
golubX <- as.matrix(golub[,-1])
### learningsets
set.seed(111)
lset <- GenerateLearningsets(y=golubY, method = "CV", fold=5, strat =TRUE)
### tuning after gene selection with the t.test
tuneres <- tune(X = golubX, y = golubY, learningsets = lset,
              genesellist = list(method = "t.test"),
              classifier=compBoostCMA, nbgene = 100,
              grids = list(mstop = c(50, 100, 250, 500, 1000)))
### inspect results
show(tuneres)
best(tuneres)
plot(tuneres, iter = 3)

## End(Not run)
```

tune-methods *Hyperparameter tuning for classifiers*

Description

Performs hyperparameter tuning for the following signatures:

Methods

X = "matrix", y = "numeric", f = "missing" signature 1

X = "matrix", y = "factor", f = "missing" signature 2

X = "data.frame", y = "missing", f = "formula" signature 3

X = "ExpressionSet", y = "character", f = "missing" signature 4

For further argument and output information, consult tune.

tuningresult-class *"tuningresult"*

Description

Object returned by the function tune

Slots

hypergrid: A data.frame representing the grid of values that were tried and evaluated. The number of columns equals the number of tuned hyperparameters and the number rows equals the number of all possible combinations of the discrete grids.

tuneres: A list whose lengths equals the number of different learningsets for which tuning has been performed and whose elements are numeric vectors with length equal to the number of rows of hypergrid (s.above), containing the misclassifcation rate belonging to the respective hyperparameter/hyperparameter combination. In order to to get an overview about the best hyperparmeter/hyperparameter combination, use the convenience method best

method: Name of the classifier that has been tuned.

fold: Number of cross-validation fold used for tuning, s. argument of the same name in tune

Methods

show Use show(tuninresult-object) for brief information.

best Use best(tuningresult-object) to see which hyperparameter/hyperparameter combination has performed best in terms of the misclassification rate, s. best,tuningresult-method

plot Use plot(tuningresult-object, iter, which) to display the performance of hyperparameter/hyperparameter combinations graphically, either as one-dimensional or as two-dimensional (contour) plot, s. plot,tuningresult-method

Author(s)

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See Also

tune

---

varseloutput-class *"varseloutput"*

Description

An object returned by the functions described in filter, usually not created directly by the user.

Slots

varsel: numeric vector of variable importance measures, e.g. absolute of genewise statistics.

Methods

No methods are currently defined.

Author(s)

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See Also

filter, clvarseloutput

---

weighted.mcr *Tuning / Selection bias correction*

Description

Performs subsampling for several classifiers or a single classifiers with different tuning parameter values or numbers of selected genes. Eventually, a specific procedure for correcting for the tuning or selection bias, which is caused by optimal selection of classifiers or tuning parameters, is applied.

Usage

```
weighted.mcr(classifiers,parameters,nbgenes,sel.method,X,y,portion,niter=100,shrinkage=F)
```

Arguments

classifiers	A character vector of the several CMA classifiers that shall be used. If the same classifier shall be used with different tuning parameters it must appear several times in this vector.
parameters	A character containing the tuning parameter values corresponding to the classification methods in classifiers. Must have the same length as classifiers.
nbgenes	A numeric vector indicating how many variables shall be selected by sel.method for the corresponding classifier. Must have the same length as classifiers.
sel.method	The CMA-method (represented as a string) that shall be applied for variable selection. If this parameter is set to 'none' no variable selection is performed.
X	The matrix of gene expression data. Can be one of the following. Rows correspond to observations, columns to variables.
y	Class labels. Can be one of the following: • A numeric vector. • A factor. **WARNING**: The class labels will be re-coded to range from 0 to K-1, where K is the total number of different classes in the learning set.
portion	A numeric value which indicates the portion of observations that will be used for training the classifiers.
niter	The number of subsampling iterations.
shrinkage	A logical value indicating whether shrinkage (WMCS) shall be applied.

Details

The algorithm tries to avoid the additional computational costs of a nested cross validation by estimating the corrected misclassification rate of the best classifier by a weighted mean of all classifiers included in the subsampling approach.

Value

An object of class wmcr.result which provides the corrected and uncorrected misclassification rate of the best classifier as well as weights and misclassifcation rates for all classifiers used in the subsampling approach.

Author(s)

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References

Bernau Ch., Augustin, Th. and Boulesteix, A.-L. (2011): Correcting the optimally selected resampling-based error rate: A smooth analytical alternative to nested cross-validation. Department of Statistics: Technical Reports, Nr. 105.

See Also

wmc,classification,GeneSelection, tune, evaluation,

Examples

```
#inputs
classifiers<-rep('knnCMA',7)
nbgenes<-rep(50,7)
parameters<-c('k=1','k=3','k=5','k=7','k=9','k=11','k=13')
portion<-0.8
niter<-100
data(golub)
X<-as.matrix(golub[,-1])
y<-golub[,1]
sel.method<-'t.test'
#function call
wmcr<-weighted.mcr(classifiers=classifiers,parameters=parameters,nbgenes=nbgenes,sel.method=sel.method,X=X,
```

`weighted.mcr-methods` *General method for tuning / selection bias correction*

Description

Perform tuning / selection bias correction in subsampling for the following signatures:

Methods

classifiers="character",parameters="character",nbgenes="numeric",sel.method="character",X = "matrix", y =
signature 1

classifiers="character",parameters="character",nbgenes="numeric",sel.method="character",X = "matrix", y =
signature 2

classifiers="character",parameters="character",nbgenes="missing",sel.method="character",X = "matrix", y =
signature 3

For further argument and output information, consult `weighted.mcr`.

`wmc` *Tuning / Selection bias correction based on matrix of subsampling fold errors*

Description

Perform tuning / selection bias correction for a matrix of subsampling fold errors.

Usage

```
wmc(mcr.m,n.tr,n.ts,shrinkage=F)
```

Arguments

`mcr.m`	A matrix of resampling fold errors. Columns correspond the the fold errors of a single classifier.
`n.tr`	Number of observations in the resampling training sets.
`n.ts`	Number of observations in the resampling test sets.
`shrinkage`	A logical value indicating whether shrinkage (WMCS) shall be applied.

Details

The algorithm tries to avoid the additional computational costs of a nested cross validation by estimating the corrected misclassification rate of the best classifier by a weighted mean of all classifiers included in the subsampling approach.

Value

A list containing the corrected misclassification rate, the index of the best method and a logical value indicating whether shrinkage has been applied.

Author(s)

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References

Bernau Ch., Augustin, Th. and Boulesteix, A.-L. (2011): Correcting the optimally selected resampling-based error rate: A smooth analytical alternative to nested cross-validation. Department of Statistics: Technical Reports, Nr. 105.

See Also

weighted.mcr,classification,GeneSelection, tune, evaluation,

---

wmc-methods *General method for tuning / selection bias correction based on a matrix of subsampling fold errors.*

Description

Perform tuning / selection bias correction for a matrix of subsampling fold errors for the following signature:

Methods

mcr.m="matrix",n.tr="numeric",n.ts="numeric" signature 1

For further argument and output information, consult wmc.

`wmcr.result-class` *"wmcr.result"*

Description

Object returned by function `weighted.mcr`.

Slots

`corrected.mcr`: The corrected misclassification rate for the best method.

`best.method`: The method which performed best in the subsampling approach.

`mcrs`: Misclassification rates of all classifiers used in the subsampling approach.

`weights`: The weights used for the different classifiers in the correction method.

`cov`: Estimated covariance matrix for the misclassification rates of the different classifiers.

`uncorrected.mcr` The uncorrected misclassification rate of the best method.

`ranges` Minimum and maximal mean misclassification rates as well as the theoretical bound for nested cross validation (averaging over foldwise minima or maxima respectively).

`mcr.m` matrix of resampling fold errors, columns correspond to the fold errors of a single classifier

`shrinkage` a logical value indicating whether shrinkage (WMCS) has been aplied.

Methods

show Use `show(wmcr.result-object)` for brief information

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See Also

`weighted.mcr`

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