Package 'classyfire'

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Description A collection of functions for the creation and application of highly optimised, robustly evaluated ensembles of support vector machines (SVMs). The package takes care of training individual SVM classifiers using a fast parallel heuristic algorithm, and combines individual classifiers into ensembles. Robust metrics of classification performance are offered by bootstrap resampling and permutation testing.	
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	bies

Description

The aim of the classyfire package is to improve the quality of multivariate classification projects by making a state-of-the-art multivariate classification workflow available to everyone. Classyfire achieves this by providing powerful functions which automate as much of the classifier building and testing as possible. However, to avoid these functions becoming impenetrable black boxes, detailed information is provided about how these functions work, and full access is provided to the internals of all classifiers that are produced.

Details

Package: classyfire
Type: Package
Version: 1.0
Date: 2014-09-03

License: GPL (>= 2)

Author(s)

Adapted functionality by Eleni Chatzimichali (ea.chatzimichali@gmail.com)

Author of the SVM functions: David Meyer (<David.Meyer@R-project.org>)

(based on C/C++-code by Chih-Chung Chang and Chih-Jen Lin)

Author of Scilab neldermead module: Michael Baudin (INRIA - Digiteo)

Author of Scilab R adaptation: Sebastien Bihorel (<sb.pmlab@gmail.com>)

Authors of bootstrap functions: Angelo Canty and Brian Ripley (originally by Angelo Canty for S)

References

There are many references explaining the concepts behind the functionality of this package. Among them are :

Chang, Chih-Chung and Lin, Chih-Jen:

LIBSVM: a library for Support Vector Machines

http://www.csie.ntu.edu.tw/~cjlin/libsvm

Exact formulations of models, algorithms, etc. can be found in the document:

Chang, Chih-Chung and Lin, Chih-Jen:

LIBSVM: a library for Support Vector Machines

http://www.csie.ntu.edu.tw/~cjlin/papers/libsvm.ps.gz

More implementation details and speed benchmarks can be found on:

Rong-En Fan and Pai-Hsune Chen and Chih-Jen Lin:

Working Set Selection Using the Second Order Information for Training SVM

http://www.csie.ntu.edu.tw/~cjlin/papers/quadworkset.pdf

Spendley, W. and Hext, G. R. and Himsworth, F. R. Sequential Application of Simplex Designs in Optimisation and Evolutionary Operation American Statistical Association and American Society for Quality, 1962

Nelder, J. A. and Mead, R. A Simplex Method for Function Minimization The Computer Journal, 1965

C. T. Kelley

Iterative Methods for Optimization

SIAM Frontiers in Applied Mathematics, 1999

A. C. Davison and D. V. Hinkley Bootstrap Methods and Their Applications CUP, 1997

Booth, J.G., Hall, P. and Wood, A.T.A. *Balanced importance resampling for the bootstrap.* Annals of Statistics, 21, 286-298, 1993

Davison, A.C. and Hinkley, D.V. *Bootstrap Methods and Their Application* Cambridge University Press, 1997

Efron, B. and Tibshirani, R. *An Introduction to the Bootstrap* Chapman & Hall, 1993

cfBuild

Create a highly optimised ensemble of RBF SVM classifiers

Description

The cfBuild function creates a highly optimised ensemble of radial basis function (RBF) support vector machines (SVMs). The cfBuild function takes care of all aspects of the SVM optimisation, internally splitting the supplied data into separate training and testing subsets using a bootstrapping approach coupled with a heuristic optimisation algorithm and parallel processing to minimise computation time. The ensemble object can then be used to classify newly acquired data using the cfPredict function.

Usage

Arguments

inputData The input data matrix as provided by the user (mandatory field).

The input class vector as provided by the user (mandatory field).

bootNum The number of bootstrap iterations in the optimisation process. By default, the

bootNum value is set to 100.

ensNum The number of classifiers that form the classification ensemble. By default, the

ensNum value is set to 100.

parallel Boolean value that determines parallel or sequential execution. By default set to

TRUE. For more details, see sfInit.

cpus Numeric value that provides the number of CPUs requested for the cluster. For

more details, see sfInit.

type The type of cluster. It can take the values 'SOCK', 'MPI', 'PVM' or 'NWS'.

By default, type is equal to 'SOCK'. For more details, see sfInit.

socketHosts Host list for socket clusters. Only needed for socketmode (SOCK) and if using

more than one machines (if using only your local machine (localhost) no list is

needed). For more details, see sfInit.

... The remaining optional fields.

Details

For a given input dataset D, a random fraction of samples is removed and kept aside as an independent test set during the training process of the model. This selection of samples forms the dataset D_{test} . This test set typically comprises a third of the original samples. Using a stratified holdout approach, the test set consists of the same balance of sample classes as the initial dataset D. The remaining samples that are not selected, form the training set D_{train} . Since the test set is kept aside during the whole training process, the risk of overfitting is minimised.

In the case of bootstrapping, a bootstrap training set $D_{bootTrain}$ is created by randomly picking n samples with replacement from the training dataset D_{train} . The total size of $D_{bootTrain}$ is equal to the size of D_{train} . Since bootstrapping is based on sampling with replacement, any given sample could be present multiple times within the same bootstrap training set. The remaining samples not found in the bootstrap training set make up the bootstrap test set $D_{bootTest}$. To avoid reliance on one specific bootstrapping split, bootstrapping is repeated at least bootNum times until a clear winning parameter combination emerges.

Ultimately, the optimal parameters are used to train a new classifier with the full D_{train} dataset and test it on the independent test set D_{test} , which has been left aside during the entire optimisation process. Even though the approach described thus far generates an excellent classifier, the random selection of test samples in the initial split may have been fortunate. For a more accurate and reliable overview, the whole process should be repeated a minimum of 100 times (default value of ensNum) or until a stable average classification rate emerges. The output of this repetition consists of at least ensNum individual classification models built using the optimum parameter settings. Rather than isolating a single classifier, all individual classification models are fused into a classification ensemble.

Value

The cfBuild function returns an object in the form of an R list. The attributes of the list can be accessed by executing the attributes command. More specifically, the list of attributes includes:

testAcc The test accuracy (%CC) of a single classifier in the ensemble.

trainAcc	The train accuracy of a single classifier in the ensemble.
optGamma	Optimal gamma value for a single SVM model
optCost	Optimal cost value for a single SVM model
runTime	The execution time for a single classifier within the ensemble.
confMatr	The confusion matrix of a single classifier.
propTable	Similar to the confusion matrix, the per class (%) accuracies.
predClass	The vector of classes for the test class as predicted by the SVM model.
testClass	The vector of true classes of the test class.
missNames	In case that the names of the samples (rows) are supplied in the input data matrix, the missNames attribute returns the names of the missclassified samples.
accNames	In case that the names of the samples (rows) are supplied in the input data matrix, the accNames attribute returns the names of the correctly classified samples.
trainClass	The vector of classes used in the training of the SVM.
testData	The data matrix (individual test set) used for testing.
trainData	The data matrix (individual test set) used for training.
testSamples	The randomly selected samples (rows) that were used in this instance to create the train and test data.
boot0bj	The matrix of bootstrapped samples based on the provided bootNum.
svmModel	The created SVM model as an R object.

Note

- Data are scaled internally, usually yielding better results. The parameters of SVM-models usually *must* be tuned to yield sensible results! For more information, see function svm.
- The cfBuild function does not force an upper limit for the bootNum, ensNum and cpus parameters to the users. However, it is advisable not to use extremely high values for these parameters.

Author(s)

Adapted functionality by Eleni Chatzimichali (ea.chatzimichali@gmail.com)

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References

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Chang, Chih-Chung and Lin, Chih-Jen:

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Davison, A.C. and Hinkley, D.V. Bootstrap Methods and Their Application Cambridge University Press, 1997

Efron, B. and Tibshirani, R. *An Introduction to the Bootstrap* Chapman & Hall, 1993

See Also

cfPredict, cfPermute

cfPermute 7

```
# List of attributes available for each classifier in the ensemble
attributes(ens[[1]])
# The test accuracy of one individual classifier in the ensemble
round(ens[[1]]$testAcc, digits=2)
# The train accuracy of one individual classifier in the ensemble
round(ens[[1]]$trainAcc, digits=2)
# All the test accuracies and the average test accuracy in the ensemble
getAcc(ens)$Test
getAvgAcc(ens)$Test
# All the train accuracies and the average train accuracy in the ensemble
getAcc(ens)$Train
getAvgAcc(ens)$Train
# Randomly generate test data to find out their classes using the generated ensemble
# 400 points are selected at random, which results in 100 samples (rows).
testMatr <-matrix(runif(400)*100, ncol = ncol(irisData))</pre>
# Predict the classes of the data using the classifiers in the constructed ensemble
predRes <- cfPredict(ens, testMatr)</pre>
## End(Not run)
```

cfPermute

Permutation testing to indicate statistical significance of performance

Description

The cfPermute function performs permutation testing on a classification ensemble produced by cfBuild. This is essentially a comparison between the classification performance achieved for a given dataset and the performance that would be achieved by random chance. It therefore provides an indication of significance of the performance of a classifier.

Usage

Arguments

inputData The input data matrix as provided by the user (mandatory field).

The input class vector as provided by the user (mandatory field).

bootNum The number of bootstrap iterations during the optimisation process. By default,

the value is set to 100.

ensNum The number of classifiers that constitute the ensemble for each permutation. By

default, the value is set to 100.

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permNum The number of permutations to be executed. By default, the value is set to 100. Boolean value that determines parallel or sequential execution. By default set to parallel TRUE. For more details, see sfInit. Numeric value that provides the number of CPUs requested for the cluster. For cpus more details, see sfInit. The type of cluster. It can take the values 'SOCK', 'MPI', 'PVM' or 'NWS'. type By default, type is equal to 'SOCK'. For more details, see sfInit. Host list for socket clusters. Only needed for socketmode (SOCK) and if using socketHosts more than one machines (if using only your local machine (localhost) no list is needed). For more details, see sfInit.

progressBar Boolean value that determines whether a progress bar should be displayed. By

default set to TRUE.

Details

Permutation testing is a widely-applied process used in order to provide an indication of the statistical significance of the classification results. In a permutation test, the entries of the original class vector (inputClass) are randomly shuffled, while the class distribution is preserved. This approach destroys all the sample membership information since the samples of a permuted dataset correspond to randomly assigned classes. The whole model building process as described in cfBuild is once more repeated for the "false" (permuted) classes. In general, permutation testing should be performed at least 100 times (default value of permNum) until a stable distribution of results is obtained.

Value

The cfPermute function returns an object in the form of an R list. The attributes of the list can be accessed by executing the attributes command. More specifically, the list of attributes includes:

avgTestAcc The average test accuracy across all ensembles within each permutation itera-

The execution time for each permutation round. For more information see sysexecTime

For each permutation iteration, a new object (list) is generated by the function permList

> cfBuild using as input the initial data and the permuted class. This attribute will have the same length - the same number of elements - as the permNum attribute specified in the cfPermute function. For more information on the arguments of

the object, see cfBuild

References

Good, P. I.

Permutation, Parametric and Bootstrap Tests of Hypotheses 3rd ed, Springer-Verlag New York Inc, Dordrecht, 2006

Hesterberg, T., Moore, D. S., Monaghan, S., Clipson, A. and Epstein, R. Bootstrap methods and permutation tests

Introduction to the Practice of Statistics, vol. 5, pp. 1-70, 2005

See Also

getPerm5Num, ggPermHist

cfPredict 9

Examples

```
## Not run:
data(iris)
irisClass <- iris[,5]</pre>
irisData <- iris[,-5]</pre>
ens <- cfBuild(irisData, irisClass, bootNum = 100, ensNum = 100, parallel = TRUE,
               cpus = 4, type = "SOCK")
# Execute 5 permutation rounds; in each permutation test, an ensemble of 20 classifiers
# is constructed, each running 10 bootstrap iterations during the optimization process
permObj <- cfPermute(irisData, irisClass, bootNum = 10, ensNum = 20, permNum = 5, parallel = TRUE,</pre>
                    cpus = 4, type = "SOCK")
length(permObj)
attributes(permObj)
round(permObj$avgTestAcc, digits=2)
permObj$execTime
length(permObj$permList)
## End(Not run)
```

cfPredict

Predict the class of new data using an existing ensemble

Description

The cfPredict function uses a classification ensemble object created by cfBuild to predict the class(es) of one or more samples described by a given data matrix. The function returns the predicted classes for each sample, together with a confidence score (between 0 and 100) which equates to the percentage of SVMs within the classifier that voted for the reported class.

Usage

```
cfPredict(ensObj, newInputData)
```

Arguments

ens0bj The classification ensemble (in the form of an R list) as generated by cfBuild

newInputData A new independent dataset with unknown classes. The new dataset must have exactly the same number of columns as the inputData, passed as an argument

in cfBuild.

Value

The cfPredict function returs a matrix of the predicted classes as generated by a majority vote between the classifiers in the ensemble along with their confidence scores (the % percentage of the predicted class in the majority vote) for each sample.

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See Also

```
cfBuild
```

Examples

getAcc

Get the accuracies of a classification ensemble

Description

The getAcc function returns the test and train accuracies for all the classifiers within a classification ensemble as generated by cfBuild.

Usage

```
getAcc(ensObj)
```

Arguments

ens0bj

The classification ensemble (in the form of an R list) as generated by cfBuild

Value

The getAcc function returns a list with two named (Test and Train) vectors, equal to the overall test accuracies (%CC) and overall train accuracies of the classifiers within the ensemble. The attributes of the list can be accessed by executing the attributes command.

See Also

```
getAvgAcc
```

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Examples

getAvgAcc

Get the average accuracies of a classification ensemble

Description

The avgTestAcc function returns the average test accuracy (%CC) and average train accuracy of an ensemble of classifiers as generated by the function cfBuild.

Usage

```
getAvgAcc(ensObj)
```

Arguments

ens0bj

The classification ensemble (in the form of an R list) as generated by cfBuild

Value

The avgTestAcc function returns a list with two named (Test and Train) numerical values, equal to the average overall test accuracy (%CC) and the average overall train accuracy of the ensemble. The attributes of the list can be accessed by executing the attributes command.

See Also

getAcc

12 getConfMatr

Examples

getConfMatr

Confusion matrix summarising the performance of an ensemble

Description

The getConfMatr function returns a confusion matrix from an ensemble created by cfBuild. The matrix is populated using class predictions for test data, predictions which were obtained during the building and optimisation of the classifier. Each column of the confusion matrix represents the instances in a predicted class, while each row represents the instances in an actual class. Cells in the matrix indicate the percentage of samples predicted to belong to each class. In a perfect ensemble the diagonal elements would all be 100%.

Usage

```
getConfMatr(ensObj)
```

Arguments

ens0bj

The classification ensemble (in the form of an R list) as generated by cfBuild

Note

A graphical representation of this information is provided by ${\tt ggClassPred}$.

```
## Not run:
data(iris)
irisClass <- iris[,5]</pre>
```

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getOptParam

Get the optimal SVM hyperparameters of a classification ensemble

Description

To allow detailed reporting of the methods used to create classifiers, the getOptParam function retrieves the optimum hyperparameters for each SVM within an ensemble classifier, built using cfBuild.

Usage

```
getOptParam(ensObj)
```

Arguments

ens0bj

The classification ensemble (in the form of an R list) as generated by cfBuild

Value

Returns a matrix containing the optimal gamma and optimal cost for each SVM in the classification ensemble. For information about what these hyperparameters are and how they are determined, see the documentation for cfBuild.

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getPerm5Num

Get descriptive statistics from a permutation object

Description

The getPerm5Num function returns the "five number summary", a descriptive statistic that consists of the minimum, first (lower) quartile, median, third (upper) quartile and maximum value of a given distribution. In this case, the function is applied directly on the output of permutation testing, generated by the cfPermute function.

Usage

```
getPerm5Num(permObj)
```

Arguments

permObj

The permutation object as generated by cfPermute

Value

The getPerm5Num function returns an R object in the form of a list that contains the five number summary. The names of the returned statistics can be viewed by using the function attributes.

Examples

ggClassPred

Barplot of the per class accuracies.

Description

The ggClasPred function generates a barplot with the per class accuracies (%) for all the correctly classified and misclassified samples in the classification ensemble.

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Usage

Arguments

ensObj	The classification ensemble (in the form of an R list) as generated by cfBuild
position	The position may be equal to either "stack" or "dodge".
displayAll	Boolean value, by default set to FALSE. When displayAll= FALSE, only the percentages of correctly classified samples are displayed in the barplot. If displayAll = TRUE, the percentages of all classified and missclassified samples are depicted in the barplot.
showText	Boolean value, by default set to FALSE. If showText=TRUE, then the per class accuracies (%) for all classifiers in the ensemble are displayed in the plot.
xlabel	A sub title for the x axis (optional field).
ylabel	A sub title for the y axis (optional field).
• • •	Further arguments and graphical parameters passed to the ggplot.

```
## Not run:
data(iris)
irisClass <- iris[,5]</pre>
irisData <- iris[,-5]</pre>
\verb|ens <- cfBuild(irisData, irisClass, bootNum = 100, ensNum = 100, parallel = TRUE, \\
               cpus = 4, type = "SOCK")
\# Show the percentages of correctly classified samples in
# a barplot with or without text respectively
ggClassPred(ens)
ggClassPred(ens, showText = TRUE)
# Show the percentages of classified and missclassified samples
# in a barplot simultaneously with and without text
ggClassPred(ens, displayAll = TRUE)
ggClassPred(ens, position="stack", displayAll = TRUE)
# Alernatively, using a dodge position
ggClassPred(ens, position = "dodge", displayAll = TRUE, showText = TRUE)
## End(Not run)
```

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ggEnsHist Ensemble Histograms	ggEnsHist	Ensemble Histograms	
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Description

The ggEnsHist function generates a histogram of the ensemble results as generated by cfBuild.

Usage

```
ggEnsHist(ensObj, density = FALSE, percentiles = FALSE, mean = FALSE, median = FALSE)
```

Arguments

ensObj	The classification ensemble (in the form of an R list) as generated by cfBuild
density	Boolean value, by default equal to FALSE. If density = FALSE, the histogram depicts frequencies, the counts component of the result. Instead, for density = TRUE, probability densities are plotted.
percentiles	Boolean value, by default equal to FALSE. If percentiles = TRUE, the upper and lower percentiles of the distribution are depicted in the plot.
mean	Boolean value, by default equal to FALSE. If mean = TRUE, the mean of the distribution is depicted in the plot.
median	Boolean value, by default equal to FALSE. If median = TRUE, the median of the distribution is depicted in the plot.

See Also

ggEnsHist

```
## Not run:
data(iris)

irisClass <- iris[,5]
irisData <- iris[,-5]

ens <- cfBuild(irisData, irisClass, bootNum = 100, ensNum = 100, parallel = TRUE, cpus = 4, type = "SOCK")

ggEnsHist(ens)
ggEnsHist(ens, density = TRUE)
ggEnsHist(ens, density = TRUE, percentiles=TRUE)
ggEnsHist(ens, density = TRUE, percentiles=TRUE, mean=TRUE)
ggEnsHist(ens, density = TRUE, percentiles=TRUE, median=TRUE)

## End(Not run)</pre>
```

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ggEnsTrend	Trend of the test accuracies

Description

The ggEnsTrend function displays the average test accuracies for every new classifier added to the ensemble, as constructed by the cfBuild function.

Usage

```
ggEnsTrend(ensObj, xlabel = NULL, ylabel = NULL, showText = FALSE, xlims = NULL, ylims = NULL, ...)
```

Arguments

ensObj	The R object as generated by cfBuild
xlabel	A sub title for the x axis (optional field).
ylabel	A sub title for the y axis (optional field).
showText	Boolean value, by default set to FALSE. If showText=TRUE, then the values of all test accuracies in the ensemble are displayed in the plot.
xlims	A vector of numeric values that specifies the minimum and maximum values in the \boldsymbol{x} axis.
ylims	A vector of numeric values that specifies the minimum and maximum values in the y axis.
• • •	Further arguments and graphical parameters passed to the ggplot.

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ggPermHist	Permutation Histograms
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Description

The ggPermHist function generates a histogram of the permutation results as generated by cfPermute.

Usage

Arguments

permObj	The permutation object as generated by cfPermute
density	Boolean value, by default equal to FALSE. If density = FALSE, the histogram depicts frequencies, the counts component of the result. Instead, for density = TRUE, probability densities are plotted.
percentiles	Boolean value, by default equal to FALSE. If percentiles = TRUE, the upper and lower percentiles of the distribution are depicted in the plot.
mean	Boolean value, by default equal to FALSE. If mean = TRUE, the mean of the distribution is depicted in the plot.
median	Boolean value, by default equal to FALSE. If median = TRUE, the median of the distribution is depicted in the plot.
	Further arguments and graphical parameters passed to the ggplot.

See Also

ggEnsHist

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