Package 'ada'

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Title The R Package Ada for Stochastic Boosting

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Description Performs discrete, real, and gentle boost under both exponential and logistic loss on a given data set. The package ada provides a straightforward, well-documented, and broad boosting routine for classification, ideally suited for small to moderate-sized data sets.

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Description

'ada' is used to fit a variety stochastic boosting models for a binary response as described in *Additive Logistic Regression: A Statistical View of Boosting* by Friedman, et al. (2000).

Usage

```
ada(x,...)
## Default S3 method:
ada(x, y,test.x,test.y=NULL, loss=c("exponential","logistic"),
    type=c("discrete","real","gentle"),iter=50, nu=0.1, bag.frac=0.5,
    model.coef=TRUE,bag.shift=FALSE,max.iter=20,delta=10^(-10),
    verbose=FALSE,...,na.action=na.rpart)
```

S3 method for class 'formula'
ada(formula, data, ..., subset, na.action=na.rpart)

Arguments

х	matrix of descriptors.
У	vector of responses. 'y' may have only two unique values.
test.x	testing matrix of discriptors (optional)
test.y	vector of testing responses (optional)
loss	loss="exponential", "ada", "e" or any variation corresponds to the default boost- ing under exponential loss. loss="logistic", "l2", "l" provides boosting under lo- gistic loss.
type	type of boosting algorithm to perform. "discrete" performs discrete Boosting (default). "real" performs Real Boost. "gentle" performs Gentle Boost.
iter	number of boosting iterations to perform. Default = 50 .
nu	shrinkage parameter for boosting, default taken as 1.
bag.frac	sampling fraction for samples taken out-of-bag. This allows one to use random permutation which improves performance.
model.coef	flag to use stageweights in boosting. If FALSE then the procedure corresponds to epsilon-boosting.
bag.shift	flag to determine whether the stageweights should go to one as nu goes to zero. This only makes since if bag.frac is small. The rationale behind this parameter is discussed in (Culp et al., 2006).
max.iter	number of iterations to perform in the newton step to determine the coeficient.
delta	tolarence for convergence of the newton step to determine the coeficient.

ada

verbose	print the number of iterations necessary for convergence of a coeficient.
formula	a symbolic description of the model to be fit.
data	an optional data frame containing the variables in the model.
subset	an optional vector specifying a subset of observations to be used in the fitting
	process.
na.action	a function that indicates how to process 'NA' values. Default=na.rpart.
	arguments passed to rpart.control. For stumps, use rpart.control(maxdepth=1,cp=-1,minsplit=0 maxdepth controls the depth of trees, and cp controls the complexity of trees. The priors should also be fixed through the parms argument as discussed in the second reference.

Details

This function directly follows the algorithms listed in "Additive Logistic Regression: A Statistical View of Boosting".

When using usage 'ada(x,y)': x data can take the form data.frame or as.matrix. y data can take form data.frame, as.factor, as.matrix, as.array, or as.table. Missing values must be removed from the data prior to execution.

When using usage 'ada $(y\sim.)$ ': data must be in a data frame. Response can have factor or numeric values. Missing values can be present in the descriptor data, whenever na.action is set to any option other than na.pass.

After the model is fit, 'ada' prints a summary of the function call, the method used for boosting, the number of iterations, the final confusion matrix (observed classification vs predicted classification; labels for classes are same as in response), the error for the training set, and testing, training , and kappa estimates of the appropriate number of iterations.

A summary of this information can also be obtained with the command 'print(x)'.

Corresponding functions (Use help with summary.ada, predict.ada, ... varplot for additional information on these commands):

summary : function to print a summary of the original function call, method used for boosting, number of iterations, final confusion matrix, accuracy, and kappa statistic (a measure of agreement between the observed classification and predicted classification). 'summary' can be used for training, testing, or validation data.

predict : function to predict the response for any data set (train, test, or validation).

plot : function to plot performance of the algorithm across boosting iterations. Default plot is iteration number (x-axis) versus prediction error (y-axis) for the data set used to build the model. Function can also simultaneously produce an error plot for an external test set and a kappa plot for training and test sets.

pairs : function to produce pairwise plots of descriptors. Descriptors are arranged by decreasing frequency of selection by boosting (upper left = most frequently chosen). The color of the marker in the plot represents class membership; the Size of the marker represents predicted class probability. The larger the marker, the higher the probability of classification.

varplot : plot of variables ordered by the variable importance measure (based on improvement).

addtest : add a testing data set to the ada object, therefore the testing errors only have to be computed once.

update : add more trees to the ada object.

Value

model	The following items are the different components created by the algorithms: trees: ensamble of rpart trees used to fit the model alpha: the weights of the trees used in the final aggregate model (AdaBoost only; see references for more information) $F : F[[1]]$ corresponds to the training sum, $F[[2]]], \ldots$ corresponds to testing sums. errs : matrix of errs, training, kappa, testing 1, kappa 1, lw : last weights calculated, used by update routine
fit	The predicted classification for each observation in the orginal level of the response.
call	The function call.
nu	shrinakge parameter
type	The type of adaboost performed: 'discrete', 'real', 'logit', and 'gentle'.
confusion	The confusion matrix (True value vs. Predicted value) for the training data.
iter	The number of boosting iterations that were performed.
actual	The original response vector.

Warnings

For LogitBoost and Gentle Boost, under certain circumstances, the methods will fail to classify the data into more than one category. If this occurs, try modifying the rpart.control options such as 'minsplit', 'cp', and 'maxdepth'.

'ada' does not currently handle multiclass problems. However, there is an example in (Culp et al., 2006) that shows how to use this code in that setting. Plots and other functions are not set up for this analysis.

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References

Friedman, J. (1999). *Greedy Function Approximation: A Gradient Boosting Machine*. Technical Report, Department of Statistics, Standford University.

Friedman, J., Hastie, T., and Tibshirani, R. (2000). *Additive Logistic Regression: A statistical view of boosting*. Annals of Statistics, 28(2), 337-374.

Friedman, J. (2002). Stochastic Gradient Boosting. Coputational Statistics \& Data Analysis 38.

Culp, M., Johnson, K., Michailidis, G. (2006). *ada: an R Package for Stochastic Boosting* Journal of Statistical Software, 16.

See Also

print.ada,summary.ada,predict.ada plot.ada,pairs.ada,update.ada addtest

addtest

Examples

```
## fit discrete ada boost to a simple example
data(iris)
##drop setosa
iris[iris$Species!="setosa",]->iris
##set up testing and training data (60% for training)
n<-dim(iris)[1]</pre>
trind<-sample(1:n,floor(.6*n),FALSE)</pre>
teind<-setdiff(1:n,trind)</pre>
iris[,5]<- as.factor((levels(iris[,5])[2:3])[as.numeric(iris[,5])-1])</pre>
##fit 8-split trees
gdis<-ada(Species~.,data=iris[trind,],iter=20,nu=1,type="discrete")</pre>
##add testing data set
gdis=addtest(gdis,iris[teind,-5],iris[teind,5])
##plot gdis
plot(gdis,TRUE,TRUE)
##variable selection plot
varplot(gdis)
##pairwise plot
pairs(gdis,iris[trind,-5],maxvar=2)
```

##for many more examples refer to reference (Culp et al., 2006)

addtest

Add a test set to ada

Description

addtest updates the ada object to have additional testing errors and testing kappa accuracies for each iteration.

Usage

addtest(x,test.x,test.y, ...)

Arguments

х	object generated by the function ada.
test.x	new x data
test.y	the true labeling for this testing data
	other arguments not used by this function.

Value

updated ada object.

See Also

ada,update.ada

pairs.ada

Description

This command produces pairwise plots of the data. The data in the upper panel of pairwise plots colors the observations by observed class membership (if membership is provided). The lower panel of pairwise plots colors the observations by predicted classes. In addition, the plotting symbol is scaled by the the class probability estimate from by adaboost.

The varplot command produces a variable importance plot using the improve criteria given in the reference (Hastie et al.,2001, pg332). This is a rather standard measure for determining variable importance.

Usage

varplot(x, plot.it = TRUE, type = c("none", "scores"), max.var.show=30, ...)

Arguments

х	object generated by 'ada'.
train.data	the 'data.frame' of the orgianal data used to train the classifier. The names of this 'data.frame' must be the same as the variable names as the object generated by 'ada'. x.data is used by both the 'pairs' command. Default = NULL.
vars	a vector of variables to include for this plot. The variable number must correspond to a specific column in 'x'. For example, $vars=c(1,2)$, generates a plot for the first two columns for 'x.data'. Note: vars is only used for the 'pairs' command. Default = NULL.
maxvar	the maximum number of variables for the pairwise plot. If maxvar = 5, then 'varplot' chooses the five most important variables and places these in desending order in the plot. Maxvar is only used for the 'pairs' command. Default = 10 .
test.x	an option to plot pairwise descriptors for a test data set. 'test.data' should be of type 'data.frame'. 'test.data' is only used for the 'pairs' command. Default = NULL.
test.y	the corresponding response for the test data set. If 'test.response' is not spec- ified, then the color of the symbols for the test data in the pairwise plots are black; training data are colored by class. 'test.response' is only used for the 'pairs' command. Default = NULL.

plot.ada

test.only	provides pairwise plots for test data only (test.only = TRUE). Default = FALSE. If 'test.response' is not specified, then 'test.only' is ignored. 'test.only' is only used for the 'pairs' command. Default = NULL.
col	color for plot symbols one for each class. Defualt $col=c(2,4)$ (i.e. red and blue)
pch	pch for plot set two symbols. Defualt pch=c(1,2) (i.e. circle and triangle)
	Arguments to be passed into 'pairs.default'. Do not set the upper and lower panel. This is only used for the pairs command.
plot.it	provides a plot of frequencies for each variable (plot.it = TRUE). 'plot.it' is only used for the 'varplot' command. Default = NULL.
type	if type="none" then nothing is returned. Default = "none". If type="scores", the frequencies are returned.
max.var.show	if plot.it is TRUE then this controls the number of variables shown for the plot

Details

The 'varplot' command provides a sense of variable importance–the more frequently a variable is selected for boosting, the more likely the variable contains useful information for classification. Pairwise interactions of important variables can then be visualized using 'varplot'. Note: The 'pairs' command calls the 'varplot' command.

Value

scores If type="scores" then the frequencies for each variable is returned by the varplot command.

Note

This plot was designed as tool to use with adaboost. Please send any comments or suggestions for improvement to the authors.

References

Culp, M., Johnson, K., Michailidis, G. (200X). *ada: an R Package for Boosting* Journal of Statistical Software, (XX)XX

plot.ada

Plots for Ada

Description

This function produces plots of the overall classification error at each boosting iteration for both the training and test sets. In addition, the function can produce plots of the measure of agreement (kappa) between the predicted classification and actual classification at each boosting iteration for both the training and test sets.

predict.ada

Usage

```
## S3 method for class 'ada'
plot(x, kappa = FALSE, test=FALSE, cols= rainbow(dim(x$model$errs)[2]+1),tflag=TRUE, ...)
```

Arguments

x	the object created by ada.
kappa	option for a plot of Kappa values at each iteration. kappa = TRUE produces a plot of Kappa values. Default = FALSE.
test	option for a plot of testing error values at each iteration. test=TRUE produces a plot of test values. Default=FALSE.
cols	colors used for lines to be plotted
tflag	inicates whether to include the tilte in the plot or not
	additional layout command parameter (see layout).

Value

No value returned

See Also

ada

Description

predict classifies a new set of observations from a previously built classifier. This function will provide either a vector of new classes, class probability estimates, or both.

Usage

```
## S3 method for class 'ada'
predict(object, newdata, type = c("vector", "probs", "both", "F"), n.iter=NULL,...)
```

Arguments

object	object generated by ada.
newdata	new data set to predict. This data set must be of type 'data.frame' and prediction data set is required for this approach.
type	choice for preditions. type="vector" returns the default class labels. type="prob" returns the probability class estimates. type="both" returns both the default class labels and probability class estimates. type="F" returns the ensamble average, where the class label is sign(F). This is mainly usefull for the multiclass case.

print.ada

n.iter	number of iterations to consider for the prediction. By default this is iter from the ada call (n.iter< iter)
	other arguments not used by this function.

Details

This function was modeled after predict.rpart. Furthermore, predict.rpart will be invoked to handle predictions by each tree in the ensamble.

Value

fit	a vector of fitted responses. Fit will be returned if type="vector".
probs	a matrix of class probability estimates. The first column corresponds to the first label in the 'levels' of the response. The second column corresponds to the second label in the 'levels' of the response. Probs are returned whenever type="probs".
both	returns both the vector of fitted responses and class probability estimates. The first element returns the fitted responses and will be labeled as 'class'. The second element returns the class probability estimates and will be labeled as 'probs'.
F	this is used in the multiclass case when one uses the package to perform 1 v.s. all.

Note

This function is invoked by the summary, pairs, and plot S3 generics invoked with an ada object. If an error occurs in one of the above commands then try using this command directly to track possible errors. Also, the newdata data set must be of type 'data.frame' when invoking summary, pairs, and plot.

See Also

ada.default,summary.ada,print.ada, plot.ada,pairs.ada,update.ada,addtest

print.ada

Model Information for Ada

Description

print lists the model information and final confusion matrix for submitted data.

Usage

```
## S3 method for class 'ada'
print(x, ...)
```

soldat

Arguments

х	object generated by the function ada.
	other arguments not used by this function.

Details

print produces a summary of the original function call, method used for boosting, number of iterations, final confusion matrix, error from data used to build the model, and estimates of M.

Note: any object of class ada invokes print, when printed to the screen.

Value

No value returned.

See Also

ada.default,summary.ada,predict.ada, plot.ada,pairs.ada,update.ada,addtest

soldat

Solubility Data

Description

A data set that contains information about compounds used in drug discovery. Specifically, this data set consists of 5631 compounds on which an in-house solubility screen (ability of a compound to dissolve in a water/solvent mixture) was performed.

Based on this screen, compounds were categorized as either insoluble (n=3493) or soluble (n=2138). Then, for each compound, 72 continuous, noisy structural descriptors were computed.

Usage

data(soldat)

Format

A data frame with 5631 observations on the following 73 variables. Some rows have missing data.

Examples

data(soldat)

summary.ada

Description

summary lists the model information for fitted model and final confusion matrix.

Usage

```
## S3 method for class 'ada'
summary(object, n.iter=NULL, ...)
```

Arguments

object	object generated by 'ada'.
n.iter	specific iteration to obtain the trainig and testing information at.
	other arguments not used by this function.

Details

summary produces a summary of the original function call, method used for boosting for a specific iteration, accuracy, and kappa statistic (a measure of agreement between the observed classification and predicted classification) for the training data.

In addition, if any other data set (i.e. test or validation) has been incorporated to the ada object (see addtest), summary produces analogous information.

See Also

ada,predict.ada,plot.ada,pairs.ada

update.ada

Add more trees to an ada object

Description

ada.update updates the ada object to have additional trees given a new number of iterations.

Usage

```
## S3 method for class 'ada'
update(object, x, y, test.x, test.y = NULL, n.iter, ...)
```

Arguments

object	object generated by the function ada.
х	x training data
У	training response
test.x	x testing data (optional)
test.y	the true labeling for this testing data (optional)
n.iter	new number of iterations, must be provided and n.iter>iter
	other arguments not used by this function.

Value

updated ada object.

See Also

ada.default,summary.ada,predict.ada, plot.ada,pairs.ada

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