



adabag: An R Package for Classification with Boosting and Bagging

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Abstract

Boosting and bagging are two widely used ensemble methods for classification. Their common goal is to improve the accuracy of a classifier combining single classifiers which are slightly better than random guessing. Among the family of boosting algorithms, AdaBoost (adaptive boosting) is the best known, although it is suitable only for dichotomous tasks. AdaBoost.M1 and SAMME (stagewise additive modeling using a multi-class exponential loss function) are two easy and natural extensions to the general case of two or more classes. In this paper, the **adabag** R package is introduced. This version implements AdaBoost.M1, SAMME and bagging algorithms with classification trees as base classifiers. Once the ensembles have been trained, they can be used to predict the class of new samples. The accuracy of these classifiers can be estimated in a separated data set or through cross validation. Moreover, the evolution of the error as the ensemble grows can be analysed and the ensemble can be pruned. In addition, the margin in the class prediction and the probability of each class for the observations can be calculated. Finally, several classic examples in classification literature are shown to illustrate the use of this package.

Keywords: AdaBoost.M1, SAMME, bagging, R program, classification, classification trees.

1. Introduction

During the last decades, several new ensemble classification methods based in the tree structure have been developed. In this paper, the package **adabag** for R (R Core Team 2013) is described, which implements two of the most popular methods for ensembles of trees: boosting and bagging. The main difference between these two ensemble methods is that while boosting constructs its base classifiers in sequence, updating a distribution over the training examples to create each base classifier, bagging (Breiman 1996) combines the individual classifiers built

in bootstrap replicates of the training set. Boosting is a family of algorithms and two of them are implemented here: AdaBoost.M1 (Freund and Schapire 1996) and SAMME (Zhu, Zou, Rosset, and Hastie 2009). To the best of our knowledge, the SAMME algorithm is not available in any other R package.

The package **adabag** 3.2, available from the Comprehensive R Archive Network at <http://CRAN.R-project.org/package=adabag>, is the current update of **adabag** that changes the measure of relative importance of the predictor variables using the gain of the Gini index given by a variable in a tree and, in the case of the **boosting** function, the weight of this tree. For this goal, the **varImp** function of the **caret** package (Kuhn 2008, 2012) is used to get the gain of the Gini index of the variables in each tree.

Previously, the version 3.0 introduced four important new features: AdaBoost-SAMME is implemented; a new function **errorevol** shows the error of the ensembles according to the number of iterations; the ensembles can be pruned using the option **newmfinal** in the corresponding **predict** function; and the posterior probability of each class for every observation can be obtained. In addition, the version 2.0 incorporated the function **margins** to calculate the margins for the classifiers.

Since the first version of this package, in 2006, it has been used in several classification tasks from very different scientific fields such as: economics and finance (Alfaro, García, Gámez, and Elizondo 2008; Chrzanowska, Alfaro, and Witkowska 2009; De Bock and Van den Poel 2011), automated content analysis (Stewart and Zhukov 2009), interpreting signals out-of-control in quality control (Alfaro, Alfaro, Gámez, and García 2009), advances in machine learning (De Bock, Coussemment, and Van den Poel 2010; Kreml and Hofer 2008). Moreover, **adabag** is used in the R package **digeR** (Fan, Murphy, and Watson 2012) and at least in two R manuals (Maindonald and Braun 2010; Torgo 2010).

Apart from **adabag**, nowadays there are several R packages dealing with boosting methods. Among them, the most widely used are **ada** (Culp, Johnson, and Michailidis 2012), **gbm** (Ridgeway 2013) and **mboost** (Bühlmann and Hothorn 2007; Hothorn *et al.* 2013). They are really useful and well-documented packages. However, it seems that they are more focused on boosting for regression and dichotomous classification. For a more detailed revision of boosting packages see the intriguing CRAN Task View: “Machine Learning & Statistical Learning” maintained by Hothorn (2013).

The paper is organized as follows. In Section 2 a brief description of the ensemble algorithms AdaBoost.M1, SAMME and bagging is given. Section 3 explains the package functions. There are eight functions, three of them are specific for each ensemble family and two of them are common for all methods. In addition, all the functions are illustrated through a well-known classification problem, the **iris** example. This data set, although very useful for academic purposes, is too simple. Thus, Section 4 is dedicated to provide a deep insight into the working of the package through two more complex classification data sets. Finally, some concluding remarks are drawn in Section 5.

2. Algorithms

In this section a brief description of boosting and bagging algorithms is given. Their common goal is to improve the accuracy of the ensemble, combining single classifiers which are as precise and different as possible. In both cases, heterogeneity is introduced by modifying the

training set where the individual classifiers are built. However, the base classifier of each boosting iteration depends on all the previous ones through the weight updating process, whereas in bagging they are independent. In addition, the final boosting ensemble uses weighted majority vote while bagging uses a simple majority vote.

2.1. Boosting

Boosting is a method that makes maximum use of a classifier by improving its accuracy. The classifier method is used as a subroutine to build an extremely accurate classifier in the training set. Boosting applies the classification system repeatedly on the training data, but in each step the learning attention is focused on different examples of this set using adaptive weights, $w_b(i)$. Once the process has finished, the single classifiers obtained are combined into a final, highly accurate classifier in the training set. The final classifier therefore usually achieves a high degree of accuracy in the test set, as various authors have shown both theoretically and empirically (Banfield, Hall, Bowyer, and Kegelmeyer 2007; Bauer and Kohavi 1999; Dietterich 2000; Freund and Schapire 1997).

Even though there are several versions of the boosting algorithms (Schapire and Freund 2012; Friedman, Hastie, and Tibshirani 2000), the best known is AdaBoost (Freund and Schapire 1996). However, it can be only applied to binary classification problems. Among the versions of boosting algorithms for multiclass classification problems (Mukherjee and Schapire 2011), two of the most simple and natural extensions of AdaBoost have been chosen, which are called AdaBoost.M1 and SAMME.

Firstly, the AdaBoost.M1 algorithm can be described as follows. Given a training set $\mathbf{T}_n = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_i, y_i), \dots, (\mathbf{x}_n, y_n)\}$ where y_i takes values in $1, 2, \dots, k$. The weight $w_b(i)$ is assigned to each observation x_i and is initially set to $1/n$. This value will be updated after each step. A basic classifier, $C_b(\mathbf{x}_i)$, is built on this new training set (\mathbf{T}_b) and is applied to every training example. The error of this classifier is represented by e_b and is calculated as

$$e_b = \sum_{i=1}^n w_b(i) \mathbf{I}(C_b(\mathbf{x}_i) \neq y_i) \quad (1)$$

where $\mathbf{I}(\cdot)$ is the indicator function which outputs 1 if the inner expression is true and 0 otherwise.

From the error of the classifier in the b -th iteration, the constant α_b is calculated and used for weight updating. Specifically, according to Freund and Schapire, $\alpha_b = \ln((1 - e_b)/e_b)$. However, Breiman (Breiman 1998) uses $\alpha_b = 1/2 \ln((1 - e_b)/e_b)$. Anyway, the new weight for the $(b + 1)$ -th iteration will be

$$w_{b+1}(i) = w_b(i) \exp(\alpha_b \mathbf{I}(C_b(\mathbf{x}_i) \neq y_i)) \quad (2)$$

Later, the calculated weights are normalized to sum one. Consequently, the weights of the wrongly classified observations are increased, and the weights of the rightly classified are decreased, forcing the classifier built in the next iteration to focus on the hardest examples. Moreover, differences in weight updating are greater when the error of the single classifier is low because if the classifier achieves a high accuracy then the few mistakes take on more importance. Therefore, the alpha constant can be interpreted as a learning rate calculated as a function of the error made in each step. Moreover, this constant is also used in the final decision rule giving more importance to the individual classifiers that made a lower error.

-
1. Start with $w_b(i) = 1/n$, $i = 1, 2, \dots, n$
 2. Repeat for $b = 1, 2, \dots, B$
 - a) Fit the classifier $C_b(\mathbf{x}_i) = \{1, 2, \dots, k\}$ using weights $w_b(i)$ on \mathbf{T}_b
 - b) Compute: $e_b = \sum_{i=1}^n w_b(i) \mathbf{I}(C_b(\mathbf{x}_i) \neq y_i)$ and $\alpha_b = 1/2 \ln((1 - e_b)/e_b)$
 - c) Update the weights $w_{b+1}(i) = w_b(i) \exp(\alpha_b \mathbf{I}(C_b(\mathbf{x}_i) \neq y_i))$ and normalize them
 3. Output the final classifier $C_f(\mathbf{x}_i) = \arg \max_{j \in Y} \sum_{b=1}^B \alpha_b \mathbf{I}(C_b(\mathbf{x}_i) = j)$
-

Table 1: AdaBoost.M1 algorithm.

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1. Start with $w_b(i) = 1/n$, $i = 1, 2, \dots, n$
 2. Repeat for $b = 1, 2, \dots, B$
 - a) Fit the classifier $C_b(\mathbf{x}_i) = \{1, 2, \dots, k\}$ using weights $w_b(i)$ on \mathbf{T}_b
 - b) Compute: $e_b = \sum_{i=1}^n w_b(i) \mathbf{I}(C_b(\mathbf{x}_i) \neq y_i)$ and $\alpha_b = \ln((1 - e_b)/e_b) + \ln(k - 1)$
 - c) Update the weights $w_{b+1}(i) = w_b(i) \exp(\alpha_b \mathbf{I}(C_b(\mathbf{x}_i) \neq y_i))$ and normalize them
 3. Output the final classifier $C_f(\mathbf{x}_i) = \arg \max_{j \in Y} \sum_{b=1}^B \alpha_b \mathbf{I}(C_b(\mathbf{x}_i) = j)$
-

Table 2: SAMME algorithm.

This process is repeated every step for $b = 1, \dots, B$. Finally, the ensemble classifier calculates, for each class, the weighted sum of its votes. Therefore, the class with the highest vote is assigned. Specifically,

$$C_f(\mathbf{x}_i) = \arg \max_{j \in Y} \sum_{b=1}^B \alpha_b \mathbf{I}(C_b(\mathbf{x}_i) = j) \quad (3)$$

Table 1 shows the complete AdaBoost.M1 pseudocode.

SAMME, the second boosting algorithm implemented here, is summarized in Table 2. It is worth mentioning that the only difference between this algorithm and AdaBoost.M1 is the way in which the alpha constant is calculated, because the number of classes is taken into account in this case. Due to this modification, the SAMME algorithm only needs that $1 - e_b > 1/k$ in order for the alpha constant to be positive and the weight updating follows the right direction. That is to say, the accuracy of each weak classifier should be better than the random guess ($1/k$) instead of $1/2$, which would be an appropriate requirement for the two class case but very demanding for the multi-class one.

2.2. Bagging

Bagging is a method that combines bootstrapping and aggregating (Table 3). If the bootstrap estimate of the data distribution parameters is more accurate and robust than the traditional one, then a similar method can be used to achieve, after combining them, a classifier with

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1. Repeat for $b = 1, 2, \dots, B$
 - a) Take a bootstrap replicate \mathbf{T}_b of the training set \mathbf{T}_n
 - b) Construct a single classifier $C_b(\mathbf{x}_i) = \{1, 2, \dots, k\}$ in \mathbf{T}_b
 2. Combine the basic classifiers $C_b(\mathbf{x}_i)$, $b = 1, 2, \dots, B$ by the majority vote (the most often predicted class) to the final decision rule $C_f(\mathbf{x}_i) = \arg \max_{j \in Y} \sum_{b=1}^B \mathbf{I}(C_b(\mathbf{x}_i) = j)$
-

Table 3: Bagging algorithm.

better properties.

On the basis of the training set (\mathbf{T}_n), B bootstrap samples (\mathbf{T}_b) are obtained, where $b = 1, 2, \dots, B$. These bootstrap samples are obtained by drawing with replacement the same number of elements than the original set (n in this case). In some of these bootstrap samples, the presence of noisy observations may be eliminated or at least reduced, (as there is a lower proportion of noisy than non-noisy examples) so the classifiers built in these sets will have a better behavior than the classifier built in the original set. Therefore, bagging can be really useful to build a better classifier when there are noisy observations in the training set.

The ensemble usually achieves better results than the single classifiers used to build the final classifier. This can be understood since combining the basic classifiers also combines the advantages of each one in the final ensemble.

2.3. The margin

In the boosting literature, the concept of margin (Schapire, Freund, Bartlett, and Lee 1998) is important. The margin for an object is intuitively related to the certainty of its classification and is calculated as the difference between the support of the correct class and the maximum support of an incorrect class. For k classes, the margin of an example \mathbf{x}_i is calculated using the votes for every class j in the final ensemble, which are known as the degree of support of the different classes or posterior probabilities $\mu_j(\mathbf{x}_i)$, $j = 1, 2, \dots, k$ as

$$m(\mathbf{x}_i) = \mu_c(\mathbf{x}_i) - \max_{j \neq c} \mu_j(\mathbf{x}_i) \quad (4)$$

where c is the correct class of \mathbf{x}_i and $\sum_{j=1}^k \mu_j(\mathbf{x}_i) = 1$. All the wrongly classified examples will therefore have negative margins and those correctly classified ones will have positive margins. Correctly classified observations with a high degree of confidence will have margins close to one. On the other hand, examples with an uncertain classification will have small margins, that is to say, margins close to zero. Since a small margin is an instability symptom in the assigned class, the same example could be assigned to different classes by similar classifiers. For visualization purposes, Kuncheva (2004) uses margin distribution graphs showing the cumulative distribution of the margins for a given data set. The x-axis is the margin (m) and the y-axis is the number of points where the margin is less than or equal to m . Ideally, all points should be classified correctly so that all the margins are positive. If all the points have been classified correctly and with the maximum possible certainty, the cumulative graph will be a single vertical line at $m = 1$.

3. Functions

In this section, the functions of the **adabag** package in R are explained. As mentioned before, it implements AdaBoost.M1, SAMME and bagging with classification and regression trees, (CART, Breiman, Friedman, Olshenn, and Stone 1984) as base classifiers using the **rpart** package (Therneau, Atkinson, and Ripley 2013). Here boosted or bagged trees are used, although these algorithms can be used with other basic classifiers. Therefore, ahead in the paper boosting or bagging refer to boosted trees or bagged trees.

This package consists of a total of eight functions, three for each method and the **margins** and **evolerror**. The three functions for each method are: one to build the boosting (or bagging) classifier and classify the samples in the training set; one which can predict the class of new samples using the previously trained ensemble; and lastly, another which can estimate by cross validation the accuracy of these classifiers in a data set. Finally, the margin in the class prediction for each observation and the error evolution can be calculated.

3.1. The boosting, predict.boosting and boosting.cv functions

As aforementioned, there are three functions with regard to the boosting method in the **adabag** package. Firstly, the **boosting** function enables to build an ensemble classifier using AdaBoost.M1 or SAMME and assign a class to the training samples. Any function in R requires a set of initial arguments to be fixed; in this case, there are six of them. The **formula**, as in the **lm** function, spells out the dependent and independent variables. The **data** frame in which to interpret the variables named in **formula**. It collects the data to be used for training the ensemble. If the logical parameter **boos** is **TRUE** (by default), a bootstrap sample of the training set is drawn using the weight for each observation on that iteration. If **boos** is **FALSE**, every observation is used with its weight. The integer **mfinal** sets the number of iterations for which boosting is run or the number of trees to use (by default **mfinal** = 100 iterations).

If the logical argument **coeflearn** = "Breiman" (by default), then $\alpha = 1/2 \ln((1 - e_b)/e_b)$ is used. However, if **coeflearn** = "Freund", then $\alpha = \ln((1 - e_b)/e_b)$ is used. In both cases the AdaBoost.M1 algorithm is applied and **alpha** is the weight updating coefficient. On the other hand, if **coeflearn** = "Zhu", the SAMME algorithm is used with $\alpha = \ln((1 - e_b)/e_b) + \ln(k - 1)$. As above mentioned, the error of the single trees must be in the range (0, 0.5) for AdaBoost.M1, while for SAMME in the range (0, $1 - 1/k$). In the case where these assumptions are not fulfilled, Opitz and Maclin (Opitz and Maclin 1999) reset all the weights to be equal, choose appropriate values to weight these trees and restart the process. The same solution is applied here. When $e_b = 0$, the **alpha** constant is calculated using $e_b = 0.001$ and when $e_b \geq 0.5$ ($e_b \geq 1 - 1/k$ for SAMME), it is replaced by 0.499 ($0.999 - 1/k$, respectively).

Lastly, the option **control** that regulates details of the **rpart** function is also transferred to **boosting** specially to limit the size of the trees in the ensemble. See **rpart.control** for more details.

Upon applying **boosting** and training the ensemble, this function outputs an object of class **boosting**, which is a list with seven components. The first one is the **formula** used to train the ensemble. Secondly, the **trees** which have been grown along the iterations are shown. A vector which depicts the **weights** of the trees. The **votes** matrix describing, for each

observation, the number of trees that assigned it to each class, weighting each tree by its alpha coefficient. The `prob` matrix showing, for each observation, an approximation to the posterior probability achieved in each class. This estimation of the probabilities is calculated using the proportion of votes or support in the final ensemble. The `class` vector is the class predicted by the ensemble classifier. Finally, the `importance` vector returns the relative importance or contribution of each variable in the classification task.

It is worth to highlight that the `boosting` function allows quantifying the relative importance of the predictor variables. Understanding a small individual tree can be easy. However, it is more difficult to interpret the hundreds or thousands of trees used in the boosting ensemble. Therefore, to be able to quantify the contribution of the predictor variables to the discrimination is a really important advantage. The measure of importance takes into account the gain of the Gini index given by a variable in a tree and the weight of this tree in the case of boosting. For this goal, the `varImp` function of the `caret` package is used to get the gain of the Gini index of the variables in each tree.

The well-known `iris` data set is used as an example to illustrate the use of `adabag`. The package is loaded using `library("adabag")` and automatically the program calls the required packages `rpart`, `caret` and `mlbench` (Leisch and Dimitriadou 2012).

The dataset is randomly divided into two equal size sets. The training set is classified with a boosting ensemble of 10 trees of maximum depth 1 (stumps) using the code below. The list returned consists of the formula used, the 10 small trees and the weights of the trees. The lower the error of a tree, the higher its weight. In other words, the lower the error of a tree, the more relevant in the final ensemble. In this case, there is a tie among four trees with the highest weights (numbers 3, 4, 5 and 6). On the other hand, tree number 9 has the lowest weight (0.175). The matrices `votes` and `prob` show the weighted votes and probabilities that each observation (rows) receives for each class (columns). For instance, the first observation receives 2.02 votes for the first, 0.924 for the second and 0 for the third class. Therefore, the probabilities for each class are 68.62%, 31.38% and 0%, respectively, and the assigned class is "setosa" as can be seen in the `class` vector.

```
R> library("adabag")
R> data("iris")
R> train <- c(sample(1:50, 25), sample(51:100, 25), sample(101:150, 25))
R> iris.adaboost <- boosting(Species ~ ., data = iris[train, ], mfinal = 10,
+   control = rpart.control(maxdepth = 1))
R> iris.adaboost

$formula
Species ~ .

$trees
$trees[[1]]
n = 75

node), split, n, loss, yval, (yprob)
* denotes terminal node
```



```

1) root 75 46 virginica (0.29333333 0.32000000 0.38666667)
  2) Petal.Length < 4.8 44 22 setosa (0.50000000 0.50000000 0.00000000) *
  3) Petal.Length >= 4.8 31 2 virginica (0.00000000 0.06451613 0.93548387) *

```

```

$trees[[2]]
n= 75

```

```

node), split, n, loss, yval, (yprob)
      * denotes terminal node

```

```

1) root 75 40 versicolor (0.22666667 0.46666667 0.30666667)
  2) Petal.Width < 1.7 53 18 versicolor (0.32075472 0.66037736 0.01886792) *
  3) Petal.Width >= 1.7 22 0 virginica (0.00000000 0.00000000 1.00000000) *

```

```

...

```

```

$trees[[10]]
n= 75

```

```

node), split, n, loss, yval, (yprob)
      * denotes terminal node

```

```

1) root 75 42 virginica (0.21333333 0.34666667 0.44000000)
  2) Petal.Width < 1.7 46 20 versicolor (0.34782609 0.56521739 0.08695652) *
  3) Petal.Width >= 1.7 29 0 virginica (0.00000000 0.00000000 1.00000000) *

```

```

$weights
[1] 0.3168619 0.2589715 0.3465736 0.3465736 0.3465736 0.3465736 0.2306728
[8] 0.3168619 0.1751012 0.2589715

```

```

$votes
      [,1]      [,2]      [,3]
[1,] 2.0200181 0.923717 0.0000000
[2,] 2.0200181 0.923717 0.0000000
...
[25,] 2.0200181 0.923717 0.0000000
[26,] 0.6337238 1.963438 0.3465736
[27,] 0.0000000 1.732765 1.2109701
...
[50,] 0.6337238 1.788337 0.5216748
[51,] 0.0000000 1.039721 1.9040144
[52,] 0.0000000 1.039721 1.9040144
...
[74,] 0.0000000 1.039721 1.9040144
[75,] 0.0000000 1.039721 1.9040144

```

```

$prob

```



```

      [,1]      [,2]      [,3]
[1,] 0.6862092 0.3137908 0.0000000
[2,] 0.6862092 0.3137908 0.0000000
...
[25,] 0.6862092 0.3137908 0.0000000
[26,] 0.2152788 0.6669886 0.1177326
[27,] 0.0000000 0.588628 0.411372
...
[50,] 0.2152788 0.6075060 0.1772152
[51,] 0.0000000 0.3531978 0.6468022
[52,] 0.0000000 0.3531978 0.6468022
...
[74,] 0.0000000 0.3531978 0.6468022
[75,] 0.0000000 0.3531978 0.6468022

$class
 [1] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
 [6] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
[11] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
[16] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
[21] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
[26] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[31] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[36] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[41] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[46] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[51] "virginica"   "virginica"   "virginica"   "virginica"   "virginica"
[56] "virginica"   "virginica"   "virginica"   "versicolor"   "virginica"
[61] "virginica"   "virginica"   "virginica"   "virginica"   "virginica"
[66] "virginica"   "virginica"   "virginica"   "versicolor"   "versicolor"
[71] "virginica"   "virginica"   "versicolor"   "virginica"   "virginica"

$importance
Sepal.Length Sepal.Width Petal.Length Petal.Width
           0           0          83.20452          16.79548

attr("class")
[1] "boosting"

```

From the `importance` vector it can be drawn that `Petal.Length` is the most important variable, as it achieved 83.20% of the information gain. It can be graphically seen in Figure 1.

```

R> barplot(iris.adaboost$imp[order(iris.adaboost$imp, decreasing = TRUE)],
+   ylim = c(0, 100), main = "Variables Relative Importance",
+   col = "lightblue")

```

From the `iris.adaboost` object it is easy to build the confusion matrix for the training set

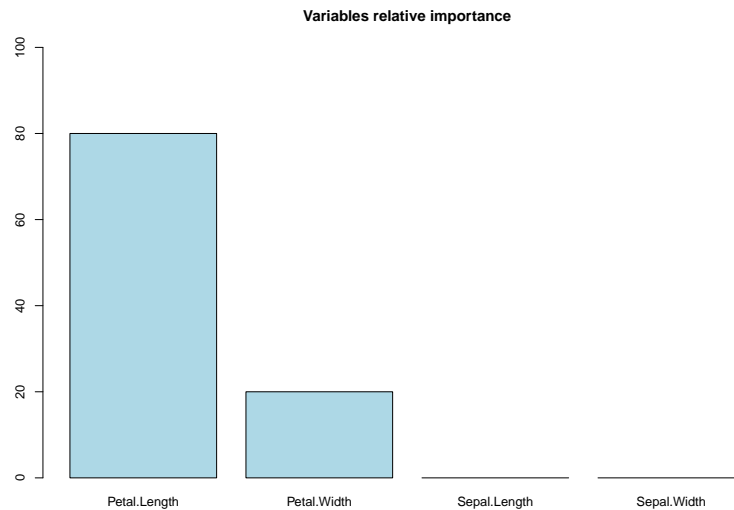


Figure 1: Variables relative importance for boosting in the `iris` example.

and calculate the error. In this case, four flowers from class `virginica` were classified as `versicolor`, so the achieved error was 5.33%.

```
R> table(iris.adaboost$class, iris$Species[train],
+       dnn = c("Predicted Class", "Observed Class"))
```

	Observed Class		
Predicted Class	setosa	versicolor	virginica
setosa	25	0	0
versicolor	0	25	4
virginica	0	0	21

```
R> 1 - sum(iris.adaboost$class == iris$Species[train]) /
+   length(iris$Species[train])
```

```
[1] 0.05333333
```

The second function `predict.boosting` matches the parameters of the generic function `predict` and adds one more (`object, newdata, newmfinal = length(objects$trees), ...`). It classifies a data frame using a fitted model `object` of class `boosting`. This is assumed to be the result of some function that produces an object with the same named components as those returned by the `boosting` function. The `newdata` argument is a data frame containing the values for which predictions are required. The predictors referred to in the right side of `formula(object)` must be present here with the same name. This way, predictions beyond the training data can be made. The `newmfinal` option fixes the number of trees of the `boosting` object to be used in the prediction. This allows the user to prune the ensemble. By default, all the trees in the object are used. Lastly, the three dots deal with further arguments passed to or from other methods.

On the other hand, this function returns an object of class `predict.boosting`, which is a list with the following six components. Four of them: `formula`, `votes`, `prob` and `class` have the same meaning as in the `boosting` output. In addition, the `confusion` matrix compares the real class with the predicted one and, lastly, the average `error` is computed.

Following with the example, the `iris.adaboost` classifier can be used to predict the class for new `iris` examples by means of the `predict.boosting` function, as it is shown below and the ensemble can also be pruned. The first four components of the output are common to the previous function output but the confusion matrix and the test data set error are here additionally provided. In this case, three virginica iris from the test data set were classified as versicolor class, so the error in this case reached 4%.

```
R> iris.predboosting <- predict.boosting(iris.adaboost,
+   newdata = iris[-train, ])
R> iris.predboosting
```

```
$formula
Species ~ .
```

```
$votes
      [,1]      [,2]      [,3]
[1,] 2.0200181 0.923717 0.0000000
[2,] 2.0200181 0.923717 0.0000000
...
[25,] 2.0200181 0.923717 0.0000000
[26,] 0.6337238 1.963438 0.3465736
[27,] 0.6337238 1.963438 0.3465736
...
[50,] 0.6337238 1.963438 0.3465736
[51,] 0.0000000 1.039721 1.9040144
[52,] 0.0000000 1.039721 1.9040144
...
[74,] 0.0000000 1.039721 1.9040144
[75,] 0.0000000 1.039721 1.9040144
```

```
$prob
      [,1]      [,2]      [,3]
[1,] 0.6862092 0.3137908 0.0000000
[2,] 0.6862092 0.3137908 0.0000000
...
[25,] 0.6862092 0.3137908 0.0000000
[26,] 0.2152788 0.6669886 0.1177326
[27,] 0.2152788 0.6669886 0.1177326
...
[50,] 0.2152788 0.6669886 0.1177326
[51,] 0.0000000 0.3531978 0.6468022
[52,] 0.0000000 0.3531978 0.6468022
...
```

```
[74,] 0.0000000 0.3531978 0.6468022
[75,] 0.0000000 0.3531978 0.6468022
```

```
$class
```

```
 [1] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
 [6] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
[11] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
[16] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
[21] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
[26] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[31] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[36] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[41] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[46] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[51] "virginica"   "virginica"   "virginica"   "virginica"   "versicolor"
[56] "virginica"   "virginica"   "virginica"   "virginica"   "virginica"
[61] "virginica"   "virginica"   "virginica"   "virginica"   "versicolor"
[66] "virginica"   "virginica"   "virginica"   "versicolor"   "virginica"
[71] "virginica"   "virginica"   "virginica"   "virginica"   "virginica"
```

```
$confusion
```

	Observed Class		
Predicted Class	setosa	versicolor	virginica
setosa	25	0	0
versicolor	0	25	3
virginica	0	0	22

```
$error
```

```
[1] 0.04
```

Finally, the third function `boosting.cv` runs v -fold cross validation with boosting. As usually in cross validation, the data are divided into v non-overlapping subsets of roughly equal size. Then, boosting is applied on $(v - 1)$ of the subsets. Lastly, predictions are made for the left out subset, and the process is repeated for each one of the v subsets.

The arguments of this function are the same seven of `boosting` and one more, an integer v , specifying the type of v -fold cross validation. The default value is 10. On the contrary, if v is set as the number of observations, leave-one-out cross validation is carried out. Besides this, every value between two and the number of observations is valid and means that one out of every v observations is left out. An object of class `boosting.cv` is supplied, which is a list with three components, `class`, `confusion` and `error`, which have been previously described in the `predict.boosting` function.

Therefore, cross validation can be used to estimate the error of the ensemble without dividing the available data set into training and test subsets. This is specially advantageous for small data sets.

Returning to the `iris` example, 10-folds cross validation is applied maintaining the number and size of the trees. The output components are: a vector with the assigned `class`, the

confusion matrix and the error mean. In this case, there are four virginica flowers classified as versicolor and three versicolor classified as virginica, so the estimated error reaches 4.67%.

```
R> iris.boostcv <- boosting.cv(Species ~ ., v = 10, data = iris, mfinal = 10,
+   control = rpart.control(maxdepth = 1))
R> iris.boostcv
```

```
$class
 [1] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
 [6] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
...
[71] "virginica"   "versicolor"  "versicolor"  "versicolor"  "versicolor"
[76] "versicolor"  "versicolor"  "virginica"   "versicolor"  "versicolor"
[81] "versicolor"  "versicolor"  "versicolor"  "virginica"   "versicolor"
...
[136] "virginica"   "virginica"   "virginica"   "versicolor"  "virginica"
[141] "virginica"   "virginica"   "virginica"   "virginica"   "virginica"
[146] "virginica"   "virginica"   "virginica"   "virginica"   "virginica"

$confusion
      Observed Class
Predicted Class setosa versicolor virginica
      setosa      50           0           0
      versicolor  0           47           4
      virginica   0           3          46

$error
[1] 0.04666667
```

3.2. The bagging, predict.bagging and bagging.cv functions

In the same way that boosting, bagging has three functions in **adabag**. The **bagging** function builds this kind of ensemble classifier and assigns the class to the training samples. The four initial parameters (**formula**, **data**, **mfinal** and **control**) have the same meaning as in the **boosting** function. It must be pointed out that unlike boosting, individual classifiers are independent among them in bagging.

This function produces an object of class **bagging**, which is a list with almost the same components as **boosting**. The only difference is the matrix with the bootstrap **samples** used along the iterations instead of the weights of the trees.

Following with the **iris** example, a bagging classifier is built with 10 trees of maximum depth 1 (stumps) using the following code for the training set. This function returns a list with the **formula** used, the 10 stumps and the matrices **votes** and **prob**. These matrices show the votes (probabilities) that each observation (rows) receives for each class (columns). For example, observation 26 receives 1, 5 and 4 votes for the first, second and third class, respectively. Thus, its probabilities are 0.1, 0.5 and 0.4, respectively, and, consequently, the assigned class is versicolor as it is shown in vector **class**. The matrix **samples** shows the selected observations in the 10 bootstrap replicates (columns) used for the ensemble.

```

R> iris.bagging <- bagging(Species ~ ., data = iris[train, ], mfinal = 10,
+   control = rpart.control(maxdepth = 1))
R> iris.bagging

$formula
Species ~ .

$trees
$trees[[1]]
n= 75

node), split, n, loss, yval, (yprob)
    * denotes terminal node

1) root 75 47 setosa (0.3733333 0.3333333 0.2933333)
   2) Petal.Length< 2.45 28  0 setosa (1.0000000 0.0000000 0.0000000) *
   3) Petal.Length>=2.45 47 22 versicolor (0.0000000 0.5319149 0.4680851) *

$trees[[2]]
n= 75

node), split, n, loss, yval, (yprob)
    * denotes terminal node

1) root 75 46 setosa (0.3866667 0.2933333 0.3200000)
   2) Petal.Length< 2.35 29  0 setosa (1.0000000 0.0000000 0.0000000) *
   3) Petal.Length>=2.35 46 22 virginica (0.0000000 0.4782609 0.5217391) *

...
$trees[[10]]
n= 75

node), split, n, loss, yval, (yprob)
    * denotes terminal node

1) root 75 45 versicolor (0.3066667 0.4000000 0.2933333)
   2) Petal.Length< 2.45 23  0 setosa (1.0000000 0.0000000 0.0000000) *
   3) Petal.Length>=2.45 52 22 versicolor (0.0000000 0.5769231 0.4230769) *

$votes
      [,1] [,2] [,3]
[1,]     9     1     0
[2,]     9     1     0
...
[25,]     9     1     0
[26,]     1     5     4
[27,]     1     5     4

```

```

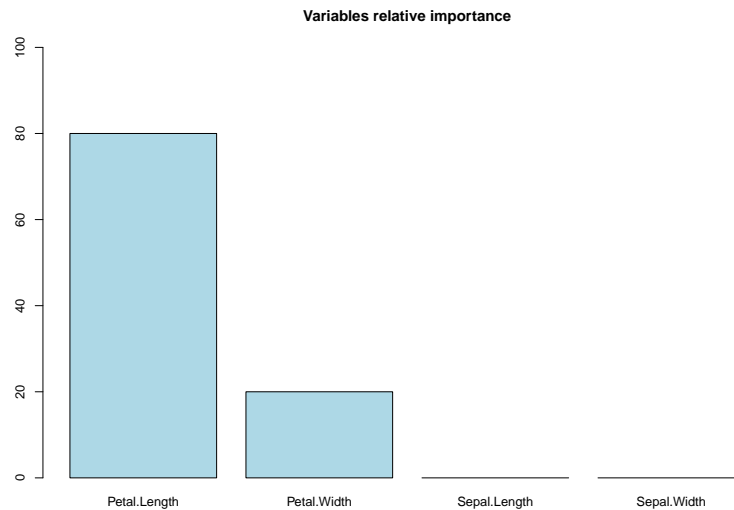
...
[50,] 1 5 4
[51,] 0 4 6
[52,] 0 4 6
...
[74,] 0 4 6
[75,] 0 4 6

$prob
      [,1] [,2] [,3]
[1,] 0.9 0.1 0
[2,] 0.9 0.1 0
...
[25,] 0.9 0.1 0
[26,] 0.1 0.5 0.4
[27,] 0.1 0.5 0.4
...
[50,] 0.1 0.5 0.4
[51,] 0 0.4 0.6
[52,] 0 0.4 0.6
...
[74,] 0 0.4 0.6
[75,] 0 0.4 0.6

$class
[1] "setosa" "setosa" "setosa" "setosa" "setosa"
[6] "setosa" "setosa" "setosa" "setosa" "setosa"
[11] "setosa" "setosa" "setosa" "setosa" "setosa"
[16] "setosa" "setosa" "setosa" "setosa" "setosa"
[21] "setosa" "setosa" "setosa" "setosa" "setosa"
[26] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[31] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[36] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[41] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[46] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[51] "virginica" "virginica" "virginica" "virginica" "virginica"
[56] "versicolor" "virginica" "versicolor" "virginica" "virginica"
[61] "virginica" "virginica" "virginica" "virginica" "virginica"
[66] "virginica" "virginica" "virginica" "virginica" "virginica"
[71] "virginica" "virginica" "virginica" "virginica" "virginica"

$samples
      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
[1,] 8 21 53 16 75 71 15 47 73 7
[2,] 58 60 65 36 51 18 29 74 65 4
[3,] 74 21 22 24 72 14 34 27 22 26
[4,] 39 26 6 16 66 29 70 32 1 28

```


Figure 2: Variables relative importance for bagging in the `iris` example.

```
[5,] 26 17 42 36 53 4 46 75 21 22
...
[71,] 3 28 13 55 53 23 64 17 27 36
[72,] 23 24 53 54 42 53 2 44 48 32
[73,] 16 17 69 12 50 15 34 30 7 42
[74,] 43 46 29 70 50 37 61 50 73 35
[75,] 45 44 13 75 19 67 49 68 1 67
```

```
$importance
Sepal.Length Sepal.Width Petal.Length Petal.Width
           0           0          79.69223          20.30777

attr("class")
[1] "bagging"
```

In line with `boosting`, the variables with the highest contributions are `Petal.Length` (79.69%) and `Petal.Width` (20.31%). On the contrary, the contribution of the other two variables is zero. It is graphically shown in Figure 2.

```
R> barplot(iris.bagging$imp[order(iris.bagging$imp, decreasing = TRUE)],
+   ylim = c(0, 100), main = "Variables Relative Importance",
+   col = "lightblue")
```

The object `iris.bagging` can be used to compute the confusion matrix and the training set error. As can be seen, only two cases are wrongly classified (two `virginica` flowers classified as `versicolor`), therefore the error is 2.67%.

```
R> table(iris.bagging$class, iris$Species[train],
+   dnn = c("Predicted Class", "Observed Class"))
```

	Observed Class		
Predicted Class	setosa	versicolor	virginica
setosa	25	0	0
versicolor	0	25	2
virginica	0	0	23

```
R> 1 - sum(iris.bagging$class == iris$Species[train]) /
+   length(iris$Species[train])
```

```
[1] 0.02666667
```

In addition, `predict.bagging` has the same arguments and values as `predict.boosting`. However, it calls a fitted `bagging` object and returns an object of class `predict.bagging`. Finally, `bagging.cv` runs v -fold cross validation with bagging. Again, the type of v -fold cross validation is added to the arguments of the `bagging` function. Moreover, the output is an object of class `bagging.cv` similar to `boosting.cv`.

The function `predict.bagging` uses the previously built object `iris.bagging` to predict the class for each observation in the test data set and to prune it, if necessary. The output is the same as in `predict.boosting`. In this case, the confusion matrix shows two virginica species classified as versicolor and vice versa, so the error is 5.33%.

```
R> iris.predbagging <- predict.bagging(iris.bagging, newdata = iris[-train, ])
R> iris.predbagging
```

```
$formula
Species ~ .
```

```
$votes
      [,1] [,2] [,3]
[1,]    9    1    0
[2,]    9    1    0
...
[26,]    1    5    4
[27,]    1    5    4
...
[74,]    0    4    6
[75,]    0    4    6
```

```
$prob
      [,1] [,2] [,3]
[1,]  0.9  0.1  0.0
[2,]  0.9  0.1  0.0
...
[26,]  0.1  0.5  0.4
[27,]  0.1  0.5  0.4
...
```

```
[74,]    0    0.4    0.6
[75,]    0    0.4    0.6
```

```
$class
```

```
 [1] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
 [6] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
[11] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
[16] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
[21] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
[26] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[31] "versicolor" "versicolor" "versicolor" "versicolor" "virginica"
[36] "versicolor" "virginica"   "versicolor" "versicolor" "versicolor"
[41] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[46] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[51] "virginica"   "virginica"   "virginica"   "virginica"   "virginica"
[56] "virginica"   "virginica"   "virginica"   "virginica"   "virginica"
[61] "virginica"   "versicolor"  "virginica"   "virginica"   "versicolor"
[66] "virginica"   "virginica"   "virginica"   "virginica"   "virginica"
[71] "virginica"   "virginica"   "virginica"   "virginica"   "virginica"
```

```
$confusion
```

	Observed Class		
Predicted Class	setosa	versicolor	virginica
setosa	25	0	0
versicolor	0	23	2
virginica	0	2	23

```
$error
```

```
[1] 0.05333333
```

Next, 10-folds cross validation is applied with bagging, maintaining the number and size of the trees. In this case, there are twelve virginica species classified as versicolor and seven versicolor classified as virginica and so, the estimated error reaches 12.66%.

```
R> iris.baggingcv <- bagging.cv(Species ~ ., v = 10, data = iris,
+   mfinal = 10, control = rpart.control(maxdepth = 1))
R> iris.baggingcv
```

```
$class
```

```
 [1] "setosa"      "setosa"      "setosa"      "setosa"      "setosa"
...
[56] "virginica"   "versicolor" "versicolor" "versicolor" "versicolor"
[61] "versicolor" "versicolor" "versicolor" "versicolor" "versicolor"
[66] "virginica"   "versicolor" "versicolor" "versicolor" "versicolor"
...
[136] "virginica"   "virginica"   "virginica"   "versicolor" "virginica"
[141] "virginica"   "virginica"   "versicolor" "virginica"   "virginica"
```

```
[146] "virginica" "virginica" "virginica" "virginica" "virginica"
```

```
$confusion
```

```

      Clase real
Clase estimada setosa versicolor virginica
      setosa      50          0          0
      versicolor  0          43         12
      virginica   0          7         38

```

```
$error
```

```
[1] 0.1266667
```

3.3. The margins and errorevol functions

Owing to its aforementioned importance the `margins` function was added to **adabag** to calculate the margins of a boosting or bagging classifier for a data frame as previously defined in Equation 4. Its usage is very easy with only two arguments:

1. `object`. This object must be the output of one of the functions `bagging`, `boosting`, `predict.bagging` or `predict.boosting`. This is assumed to be the result of some function that produces an object with at least two components named `formula` and `class`, as those returned for instance by the `bagging` function.
2. `newdata`. The same data frame used for building the object.

The output, an object of class `margins`, is a simple list with only one vector with the margins. In the following it is shown the code to calculate the margins of the bagging classifier built in the previous section, for the training and test sets, respectively. Examples with negative margins are those which have been wrongly classified. As it was stated before, there were two and four cases in each set, respectively.

```

R> iris.bagging.margins <- margins(iris.bagging, iris[train, ])
R> iris.bagging.predmargins <- margins(iris.predbagging, iris[-train, ])
R> iris.bagging.margins

```

```
$margins
```

```

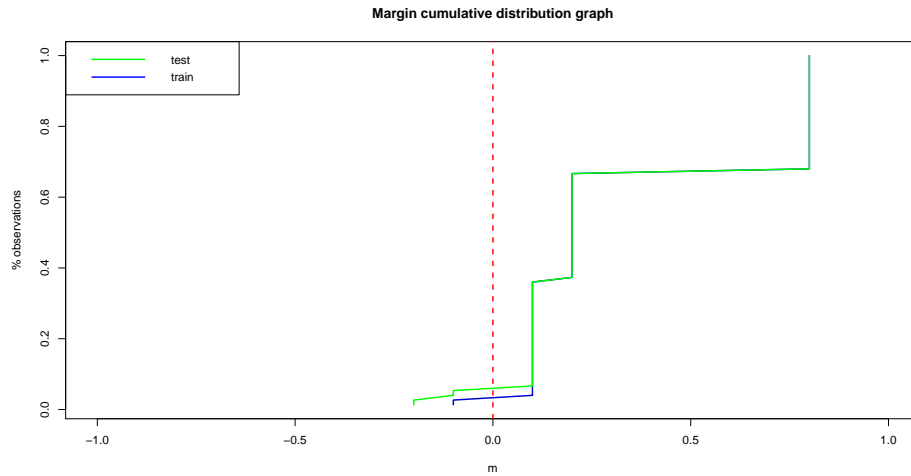
 [1] 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8
[15] 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.1 0.1 0.1
[29] 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1
[43] 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.2 0.2 0.2 0.2 -0.1
[57] 0.2 -0.1 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2
[71] 0.2 0.2 0.2 0.2 0.2

```

```
R> iris.bagging.predmargins
```

```
$margins
```

```
[1] 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8
```

Figure 3: Margins for bagging in the `iris` example.

```
[15] 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.1 0.1 0.1
[29] 0.1 0.1 0.1 0.1 0.1 0.1 -0.2 0.1 -0.2 0.1 0.1 0.1 0.1 0.1 0.1
[43] 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.2 0.2 0.2 0.2 0.2 0.2
[57] 0.2 0.2 0.2 0.2 0.2 -0.1 0.2 0.2 -0.1 0.2 0.2 0.2 0.2 0.2 0.2
[71] 0.2 0.2 0.2 0.2 0.2
```

Figure 3 shows the cumulative distribution of margins for the bagging classifier developed in this application, where the blue line corresponds to the training set and the green line to the test set. For bagging, the 2.66% of blue negative margins matches the training error and the 5.33% of the green negative ones the test error.

```
R> margins.test <- iris.bagging.predmargins[[1]]
R> margins.train <- iris.bagging.margins[[1]]
R> plot(sort(margins.train), (1:length(margins.train)) /
+   length(margins.train), type = "l", xlim = c(-1,1),
+   main = "Margin cumulative distribution graph", xlab = "m",
+   ylab = "% observations", col = "blue3", lwd = 2)
R> abline(v = 0, col = "red", lty = 2, lwd = 2)
R> lines(sort(margins.test), (1:length(margins.test)) / length(margins.test),
+   type = "l", cex = 0.5, col = "green", lwd = 2)
R> legend("topleft", c("test","train"), col = c("green", "blue"), lty = 1,
+   lwd = 2)
```

In the current version of the package, the last function is `errorevol` which calculates the error evolution of an AdaBoost.M1, AdaBoost-SAMME or bagging classifier for a data frame as the ensemble size grows. This function has the same two arguments than `margins` and outputs a list with only the vector with the error evolution. This information can be useful to see how fast bagging and boosting reduce the error of the ensemble. In addition, it can detect the presence of overfitting and, in those cases, the convenience of pruning the ensemble using the relevant `predict` function.

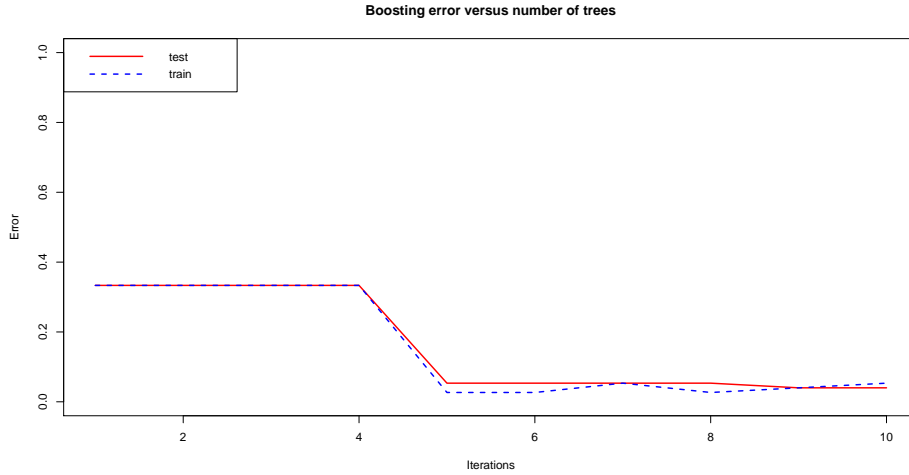


Figure 4: Error evolution for boosting in the `iris` example.

Although, due to the small size of the ensembles, this example is not the most appropriate case to show the error evolution usefulness, it is used just for demonstrative purposes.

```
R> evol.test <- errorevol(iris.adaboost, iris[-train, ])
R> evol.train <- errorevol(iris.adaboost, iris[train, ])
R> plot(evol.test$error, type = "l", ylim = c(0, 1),
+       main = "Boosting error versus number of trees", xlab = "Iterations",
+       ylab = "Error", col = "red", lwd = 2)
R> lines(evol.train$error, cex = .5, col = "blue", lty = 2, lwd = 2)
R> legend("topleft", c("test", "train"), col = c("red", "blue"), lty = 1:2,
+       lwd = 2)
```

4. Examples

The package **adabag** is now more deeply illustrated through other two classification examples. The first example shows a dichotomous classification problem using a simulated dataset previously used by [Hastie, Tibshirani, and Friedman \(2001, pp. 301–309\)](#) and [Culp, Johnson, and Michailides \(2006\)](#). The second example is a four classes data set from the UCI repository of machine learning databases ([Bache and Lichman 2013](#)). This example and `iris` are available in the **base** and **mlbench** R packages.

4.1. A dichotomous example

The two classes simulated data set consists of ten standard independent Gaussians which are used as features and the two classes defined as

$$Y = \begin{cases} 1 & \sum X_j^2 > 9.34 \\ -1 & \text{otherwise} \end{cases} \quad (5)$$

Here the value 9.34 is the median of a Chi-squared random variable with 10 degrees of freedom (sum of squares of 10 standard Gaussians). There are 2000 training and 10000 test cases,

approximately balanced. In order to enhance the comparison, stumps are also used as weak classifiers and 400 iterations are run as in [Hastie *et al.* \(2001\)](#) and [Culp *et al.* \(2006\)](#). Thus, there are only two arguments in the `boosting` function to be set. They are `coflearn` ("Breiman", "Freund" or "Zhu") and `boos` (TRUE or FALSE). Since for $k = 2$ classes the Freund and Zhu options are completely equivalent, the latter is not considered in this example. The code for running the four possible combinations of parameters is available in the additional file, and a summary of the main results is shown below.

```
R> n <- 12000
R> p <- 10
R> set.seed(100)
R> x <- matrix(rnorm(n * p), ncol = p)
R> y <- as.factor(c(-1, 1)[as.numeric(apply(x^2, 1, sum) > 9.34) + 1])
R> data <- data.frame(y, x)
R> train <- sample(1:n, 2000, FALSE)
R> formula <- y ~ .
R> vardep <- data[, as.character(formula[[2]])]
R> cntrl <- rpart.control(maxdepth = 1, minsplit = 0, cp = -1)
R> mfina1 <- 400
R> data.boosting <- boosting(formula = formula, data = data[train, ],
+   mfina1 = mfina1, coflearn = "Breiman", boos = TRUE, control = cntrl)
R> data.boostingBreimanTrue <- data.boosting
R> table(data.boosting$class, vardep[train],
+   dnn = c("Predicted Class", "Observed Class"))
```

	Observed Class	
Predicted Class	-1	1
-1	935	281
1	55	729

```
R> 1 - sum(data.boosting$class == vardep[train]) / length(vardep[train])

[1] 0.168

R> data.predboost <- predict.boosting(data.boosting, newdata = data[-train, ])
R> data.predboost$confusion
```

	Observed Class	
Predicted Class	-1	1
-1	4567	1468
1	460	3505

```
R> data.predboost$error

[1] 0.1928

R> data.boosting$imp
```


	X1	X2	X3	X4	X5	X6	X7
	10.541101	11.211198	11.195706	14.000324	8.161411	15.087848	4.827447
	X8	X9	X10				
	8.506216	7.433147	9.035603				

```
R> data.boosting <- boosting(formula = formula, data = data[train, ],
+   mfinal = mfinal, coeflearn = "Freund", boos = FALSE, control = cntrl)
R> data.boostingFreundFalse <- data.boosting
R> table(data.boosting$class, vardep[train], dnn = c("Predicted Class",
+   "Observed Class"))
```

	Observed Class	
Predicted Class	-1	1
-1	952	78
1	38	932

```
R> 1 - sum(data.boosting$class == vardep[train]) / length(vardep[train])
```

```
[1] 0.058
```

```
R> data.predboost <- predict.boosting(data.boosting, newdata = data[-train,])
R> data.predboost$confusion
```

	Observed Class	
Predicted Class	-1	1
-1	4498	613
1	529	4360

```
R> data.predboost$error
```

```
[1] 0.1142
```

```
R> data.boosting$imp
```

	X1	X2	X3	X4	X5	X6	X7
	10.071340	9.884980	10.874889	10.625273	11.287803	10.208411	8.716455
	X8	X9	X10				
	8.093104	9.706120	10.531625				

The test errors for the four aforementioned combinations on the 400-th iteration (Table 4) are 15.36%, 19.28%, 11.42% and 16.84%, respectively. Therefore, the winner combination in terms of accuracy is boosting with `coeflearn = "Freund"` and `boos = FALSE`. Results for this pair of parameters are similar to those obtained by [Hastie *et al.* \(2001\)](#) and [Culp *et al.* \(2006\)](#), 12.2% and 11.1%, respectively. In addition, the training error (5.8%) is also very close to that achieved by Culp *et al.* (6%).

Options	400 Iterations	Minimum (Iterations)
"Breiman"/FALSE	15.36	15.15 (374)
"Breiman"/TRUE	19.28	17.20 (253)
"Freund"/FALSE	11.42	11.42 (398)
"Freund"/TRUE	16.84	16.05 (325)

Table 4: Test error in percentage.

Moreover, Table 4 shows the minimum error achieved along the process and the iteration number for which this minimum value has been reached. This is possible thanks to the `errorevol` function. The pair **Freund-FALSE** (Figure 7) achieves the lowest test error and it is worth standing out that this value corresponds nearly to the end of the training process. Thus, it can be reasonably thought that the optimum value has not still been reached. The evolution of the errors for the four combinations are graphically shown in Figures 5, 6, 7 and 8, that are built running the following code for each case.

```
R> data.boosting <- data.boostingFreundFalse
R> errorevol.train <- errorevol(data.boosting, data[train, ])
R> errorevol.test <- errorevol(data.boosting, data[-train, ])
R> plot(errorevol.test[[1]], type = "l", ylim = c(0, 0.5),
+      main = "Adaboost error versus number of trees", xlab = "Iterations",
+      ylab = "Error", col = "red", lwd = 2)
R> lines(errorevol.train[[1]], cex = 0.5, col = "blue", lty = 1, lwd = 2)
R> legend("topright", c("test", "train"), col = c("red", "blue"), lty = 1,
+      lwd = 2)
R> abline(h = min(errorevol.test[[1]]), col = "red", lty = 2, lwd = 2)
R> abline(h = min(errorevol.train[[1]]), col = "blue", lty = 2, lwd = 2)
```

The option **Breiman/TRUE** (Figure 6) achieves its best result much before of the 400-th iteration and starts increasing after 253 iterations showing definitely a clear example of overfitting. This can be solved pruning the ensemble as shown next.

```
R> data.prune <- predict.boosting(data.boosting, newdata = data[-train, ],
+   newmfinal = 253)
R> data.prune$confusion
```

```

              Observed Class
Predicted Class  -1     1
              -1 4347 1040
              1   680 3933
```

```
R> data.prune$error
```

```
[1] 0.172
```

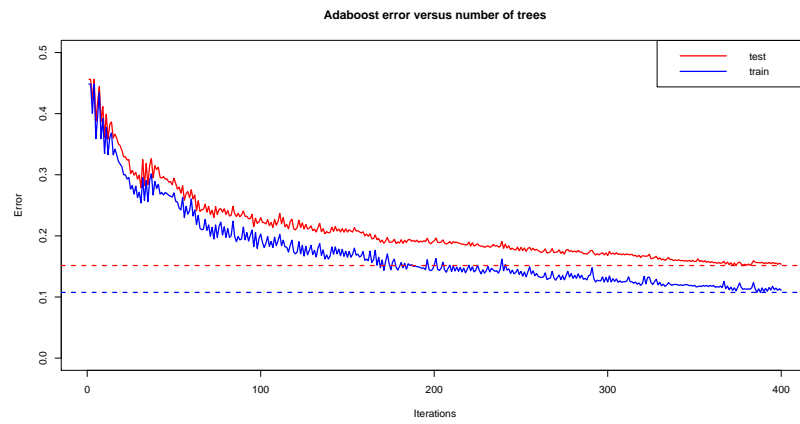


Figure 5: AdaBoost error versus number of trees with options "Breiman"/FALSE.

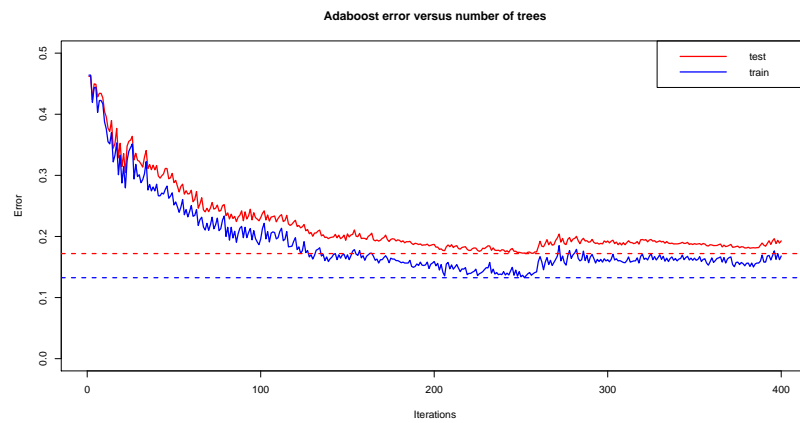


Figure 6: AdaBoost error versus number of trees with options "Breiman"/TRUE.

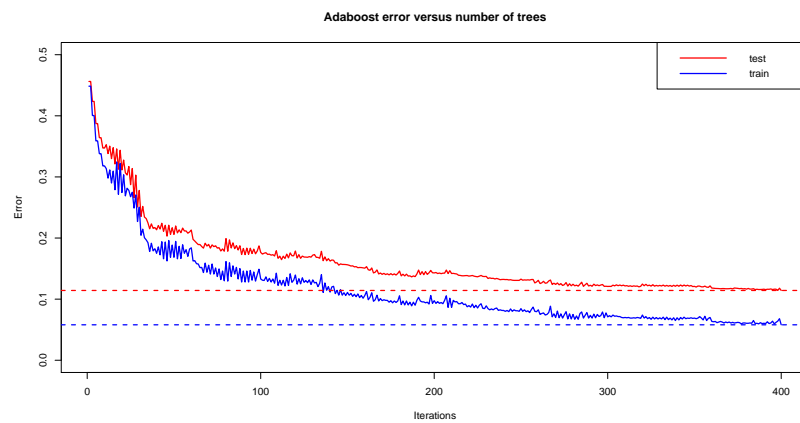


Figure 7: AdaBoost error versus number of trees with options "Freund"/FALSE.

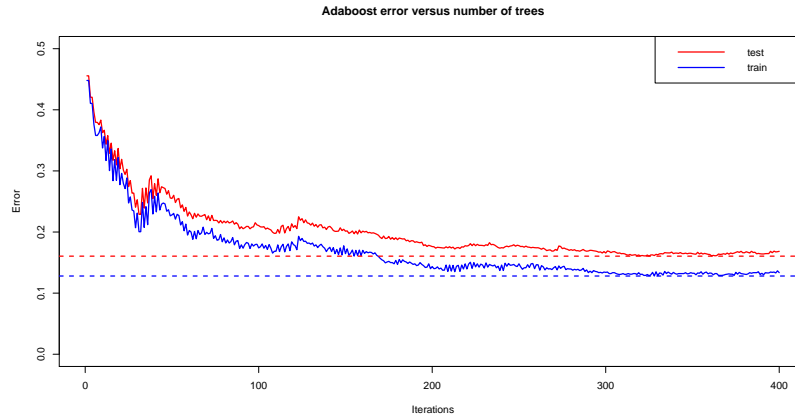


Figure 8: AdaBoost error versus number of trees with options "Freund"/TRUE.

4.2. A multiclass example

In order to show the usefulness of this package solving problems beyond the dichotomous case, a four classes example is used in this section. This problem will help to illustrate the use of the functions in problems quite more complex than the `iris` one. Specifically, the **Vehicle** data set drawn from the UCI repository is employed. This data set contains 846 samples and the purpose is to classify a given vehicle silhouette as one of four types (bus, opel, saab and van), using a set of 18 numerical features extracted from the silhouette.

With the aim of showing the advantages of using ensembles, results from a single tree are compared to those obtained with boosting and bagging. The single tree is built by means of the **rpart** package, which is automatically called when loading the **adabag** package. Due to the high number of classes, trees with maximum depth of 5 are used both in the single and the ensemble cases. The ensembles consist of 50 trees.

In order to compare the error of the four methods, 50 iterations are run and the mean result is calculated. On the other hand, to analyze some characteristics of the ensembles, as the variable relative importance and the margins, a specific model is necessary, so the model which achieves the minimum error is used.

From Table 5 it can be concluded that the single tree, with a mean test error of 32.39%, is beaten by bagging, 27.4% and particularly by Adaboost.M1 and SAMME with a much lower error, 23.94% and 24.25%, respectively. Finally, attending to the minimum error achieved by each method, the lowest test error is 17.73% by the SAMME algorithm showing its promising adaptation for the multiclass case. However, there is not a huge difference among the two boosting methods.

	CART	Bagging	AdaBoost.M1	SAMME
mean	0.3239007	0.2740426	0.2394326	0.2425532
s.d.	0.0299752	0.0274216	0.0225558	0.0292594
min.	0.2553191	0.2021277	0.1914894	0.1773050
max.	0.3971631	0.3262411	0.2872340	0.2943262

Table 5: Test error for 50 iterations.

```
R> data("Vehicle")
R> l <- length(Vehicle[, 1])
R> sub <- sample(1:l, 2 * 1/3)
R> maxdepth <- 5
R> Vehicle.rpart <- rpart(Class~., data = Vehicle[sub,], maxdepth = maxdepth)
R> Vehicle.rpart.pred <- predict(Vehicle.rpart, newdata = Vehicle,
+   type = "class")
R> 1 - sum(Vehicle.rpart.pred[sub] == Vehicle$Class[sub]) /
+   length(Vehicle$Class[sub])
```

```
[1] 0.2464539
```

```
R> tb <- table(Vehicle.rpart.pred[-sub], Vehicle$Class[-sub])
R> tb
```

	bus	opel	saab	van
bus	62	3	3	0
opel	3	26	6	1
saab	3	29	50	5
van	5	5	9	72

```
R> 1 - sum(Vehicle.rpart.pred[-sub] == Vehicle$Class[-sub]) /
+   length(Vehicle$Class[-sub])
```

```
[1] 0.2553191
```

```
R> mfinal <- 50
R> cntrl <- rpart.control(maxdepth = 5, minsplit = 0, cp = -1)
R> Vehicle.bagging <- bagging(Class ~ ., data = Vehicle[sub, ],
+   mfinal = mfinal, control = cntrl)
R> 1 - sum(Vehicle.bagging$class == Vehicle$Class[sub]) /
+   length(Vehicle$Class[sub])
```

```
[1] 0.1365248
```

```
R> Vehicle.predbagging <- predict.bagging(Vehicle.bagging,
+   newdata = Vehicle[-sub, ])
R> Vehicle.predbagging$confusion
```

	Observed Class			
Predicted Class	bus	opel	saab	van
bus	68	3	3	0
opel	1	33	9	1
saab	0	31	48	2
van	0	3	4	76

```
R> Vehicle.predbagging$error
```

```
[1] 0.2021277
```

```
R> Vehicle.adaboost <- boosting(Class ~., data = Vehicle[sub, ],
+   mfinal = mfinal, coeflearn = "Freund", boos = TRUE, control = cntrl)
R> 1 - sum(Vehicle.adaboost$class == Vehicle$Class[sub])/
+   length(Vehicle$Class[sub])
```

```
[1] 0
```

```
R> Vehicle.adaboost.pred <- predict.boosting(Vehicle.adaboost,
+   newdata = Vehicle[-sub,])
R> Vehicle.adaboost.pred$confusion
```

	Observed Class			
Predicted Class	bus	opel	saab	van
bus	68	1	0	0
opel	1	41	22	3
saab	0	21	49	0
van	1	3	2	70

```
R> Vehicle.adaboost.pred$error
```

```
[1] 0.1914894
```

```
R> Vehicle.SAMME <- boosting(Class ~ ., data = Vehicle[sub, ],
+   mfinal = mfinal, coeflearn = "Zhu", boos = TRUE, control = cntrl)
R> 1 - sum(Vehicle.SAMME$class == Vehicle$Class[sub]) /
+   length(Vehicle$Class[sub])
```

```
[1] 0
```

```
R> Vehicle.SAMME.pred <- predict.boosting(Vehicle.SAMME,
+   newdata = Vehicle[-sub, ])
R> Vehicle.SAMME.pred$confusion
```

	Observed Class			
Predicted Class	bus	opel	saab	van
bus	71	0	0	0
opel	1	43	24	1
saab	0	21	46	0
van	0	2	1	72

```
R> Vehicle.SAMME.pred$error
```

```
[1] 0.177305
```

Comparing the relative importance measure for bagging and the two boosting classifiers, they agree in pointing out the two least important variables. The Max.L.Ra has the highest contribution in bagging and AdaBoost.M1 and the second one for SAMME. Figures 9, 10 and 11 show the variables ranked by its relative importance value.

```
R> sort(Vehicle.bagging$importance, decreasing = TRUE)
```

Max.L.Ra	Sc.Var.maxis	Elong	Comp	Max.L.Rect	Sc.Var.Maxis
20.06153052	11.34898853	9.85195343	8.21094638	7.90785330	5.71291406
D.Circ	Scat.Ra	Circ	Pr.Axis.Ra	Skew.maxis	Skew.Maxis
5.47042335	5.23492044	4.62644012	4.32449318	3.84967772	3.46614732
Kurt.maxis	Kurt.Maxis	Ra.Gyr	Rad.Ra	Holl.Ra	Pr.Axis.Rect
2.98563804	2.09313159	1.70889907	1.56229729	1.54524768	0.03849798

```
R> sort(Vehicle.adaboost$importance, decreasing = TRUE)
```

Max.L.Ra	Elong	Max.L.Rect	Pr.Axis.Ra	Sc.Var.maxis	Scat.Ra
12.0048265	8.2118048	8.1391111	7.2979696	6.8809291	6.8360291
D.Circ	Sc.Var.Maxis	Comp	Skew.maxis	Rad.Ra	Ra.Gyr
6.6569366	6.3137727	6.2558542	4.9731790	4.6792429	4.5205229
Kurt.maxis	Skew.Maxis	Circ	Kurt.Maxis	Holl.Ra	Pr.Axis.Rect
4.3519975	3.6190249	3.4026665	2.9646815	2.7585392	0.1329119

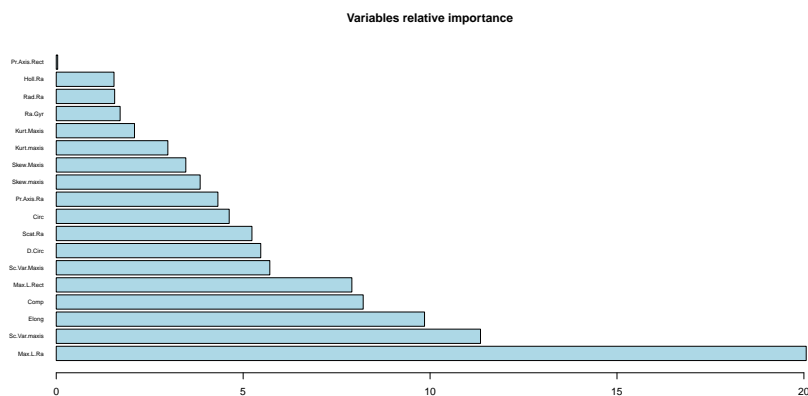
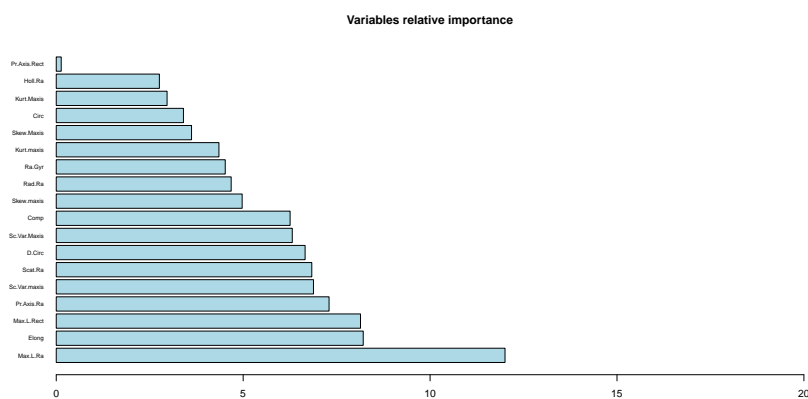
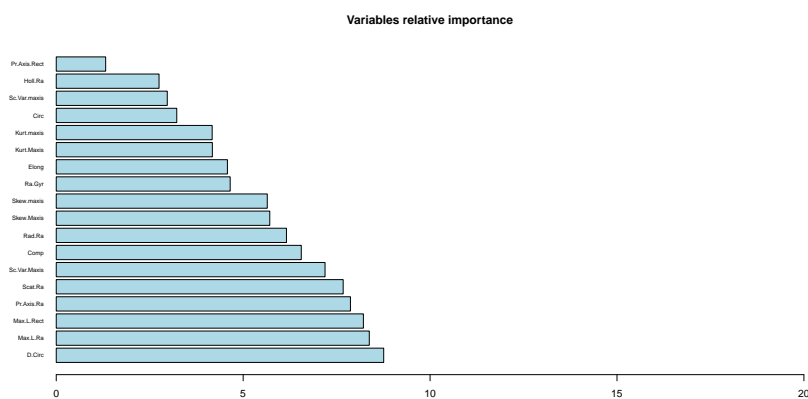
```
R> sort(Vehicle.SAMME$importance, decreasing = TRUE)
```

D.Circ	Max.L.Ra	Max.L.Rect	Pr.Axis.Ra	Scat.Ra	Sc.Var.Maxis
8.759478	8.373885	8.216298	7.869849	7.675569	7.190486
Comp	Rad.Ra	Skew.Maxis	Skew.maxis	Ra.Gyr	Elong
6.554652	6.158310	5.712122	5.644969	4.652892	4.578929
Kurt.Maxis	Kurt.maxis	Circ	Sc.Var.maxis	Holl.Ra	Pr.Axis.Rect
4.175756	4.171116	3.223761	2.969842	2.749949	1.322136

```
R> barplot(sort(Vehicle.bagging$importance, decreasing = TRUE),
+   main = "Variables Relative Importance", col = "lightblue",
+   horiz = TRUE, las = 1, cex.names = .6, xlim = c(0, 20))
```

Figures 12, 13 and 14 show the cumulative distribution of margins for the bagging and boosting classifiers developed in this application. The margin of the training set is coloured in blue and the test set in green. For AdaBoost.M1, 19.15% of green negative margins matches the test error. For SAMME, the blue line is always positive owing to the null training error. It should also be pointed out that almost 10% of the observations in bagging, for both sets, achieve the maximum margin equal to 1, which is specially outstanding taking into account the large number of classes. To be brief only the code for one of the ensembles is shown here but all of them are available in the additional file.

```
R> margins.train <- margins(Vehicle.bagging, Vehicle[sub, ])[[1]]
R> margins.test <- margins(Vehicle.bagging.pred, Vehicle[-sub, ])[[1]]
```


Figure 9: Variables relative importance for bagging in the `Vehicle` data.Figure 10: Variables relative importance for AdaBoost.M1 in the `Vehicle` data.Figure 11: Variables relative importance for SAMME in the `Vehicle` data.

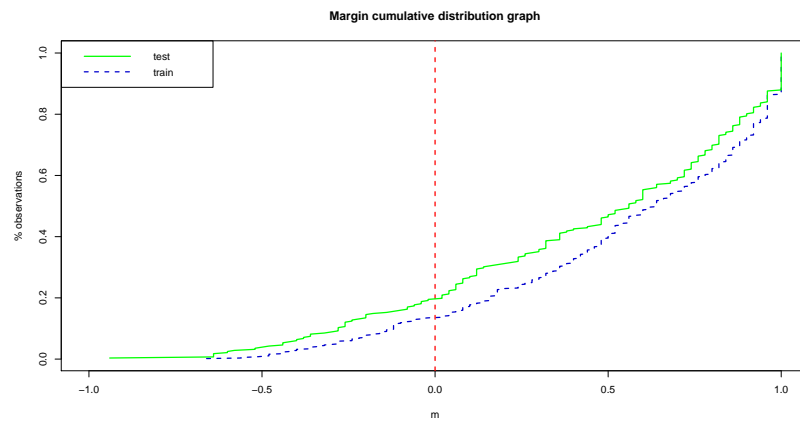


Figure 12: Margins for bagging in the **Vehicle** data.

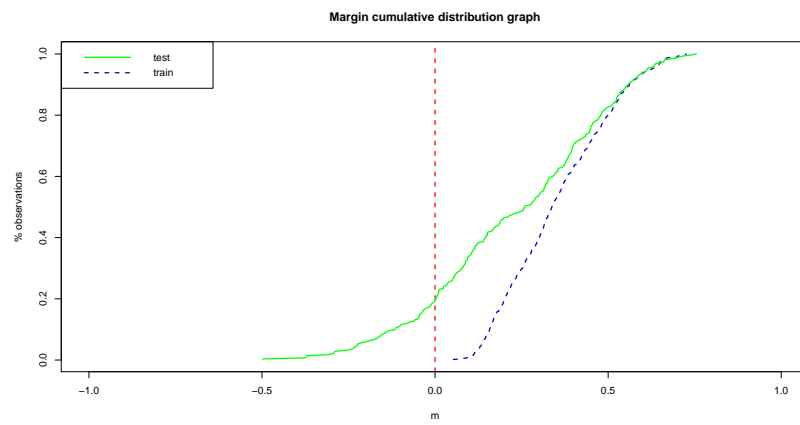


Figure 13: Margins for AdaBoost.M1 in the **Vehicle** data.

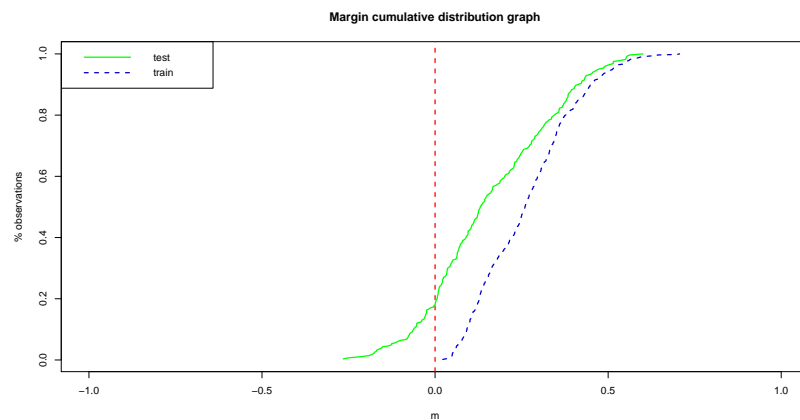


Figure 14: Margins for SAMME in the **Vehicle** data.

```

R> plot(sort(margins.train), (1:length(margins.train)) /
+   length(margins.train), type = "l", xlim = c(-1,1),
+   main = "Margin cumulative distribution graph", xlab = "m",
+   ylab = "% observations", col = "blue3", lty = 2, lwd = 2)
R> abline(v = 0, col = "red", lty = 2, lwd = 2)
R> lines(sort(margins.test), (1:length(margins.test)) / length(margins.test),
+   type = "l", cex = .5, col = "green", lwd = 2)
R> legend("topleft", c("test", "train"), col = c("green", "blue3"),
+   lty = 1:2, lwd = 2)

```

5. Summary and concluding remarks

In this paper, the R package **adabag** consisting of eight functions is described. This package implements the AdaBoost.M1, SAMME and bagging algorithms with CART trees as base classifiers, capable of handling multiclass tasks. The ensemble trained can be used for prediction on new data using the generic **predict** function. Cross validation accuracy estimations can also be achieved for these classifiers. In addition, the evolution of the error as the ensemble grows can be analysed. This can help to detect overfitting and, on the other hand, if the ensemble has not been developed enough and should keep growing. In the former case, the classifier can be pruned without rebuilding it again from the start, selecting a number of iterations of the current ensemble. Furthermore, not only the predicted class is provided, but also its margin and an approximation to the probability of all the classes.

The main functionalities of the package are illustrated here by applying them to three well-known datasets from the classification literature. The similarities and differences among the three algorithms implemented in the package are also discussed. Finally, the addition of some of the plots used here to the package, with the aim of increasing the interpretability of the results, is part of the future work.

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