Handmade AdaBoost

Álvaro Orgaz Expósito

THEORY

The aim of the *AdaBoost* algorithm is to predict the variable y (categorical for *classification* problem or continuous for *regression problem*) knowing the explanatory variables $x = \{x_1, \ldots, x_p\}$.

Firstly, you need to understand the concept of *boosting*. The idea of *boosting* is to repeatedly apply a weak algorithm on various distributions of the data (in each iteration the data is changed based on the error of the algorithm in the previous iteration, in such a way that the weak model of the iteration focuses on the incorrect previous predictions) and to ensemble the individual models into a single overall model. Then, the aim is to combine multiple models, which individually have a larger error, for getting a final model with a smaller global error.

Note: A *weak model* is any unstable predictive model whose learning algorithms are sensitive to changes in the training data. If you used complex models in each *boosting* iteration, the error would tend to 0 too fast and then the confidence of each iteration models (explained here below) would tend to infinite. It would deteriorate the final prediction.

Secondly, let's see the main steps of the *AdaBoost* algorithm, which is one of the available algorithms that use *boosting*.

1. Define the inputs $x_{[NxP]}$ and $y_{[Nx1]}$.
2. Define the number of iterations T and the weak model used in each iteration.
3. Initialize the data weights of the N observations uniformly as

$$w_i^1 = 1/N \quad for \quad i = 1, ..., N$$

4. For each iteration $t = 1, ..., T$:

   4.1 Train the weak model using the weights $w_{[Nx1]}^t$, and the inputs $x_{[NxP]}$ and $y_{[Nx1]}$. Then, compute the predictions $\hat{y}_{[Nx1]}^t$.

   4.2 Compute the global error ϵ^t of the weak model t as

   - In a *regression* problem

$$\epsilon^t = \sum_{i=1}^{N} w_i^t \times \begin{cases} 1 \;\; if \;\; \frac{|\hat{y}_i^t - y_i|}{y_i} \geq threshold \\ 0 \;\; if \;\; \frac{|\hat{y}_i^t - y_i|}{y_i} \leq threshold \end{cases}$$

     Note: *threshold* is a parameter of the model that the user defines.

   - In a *classification* problem

$$\epsilon^t = \sum_{i=1}^{N} w_i^t \times \begin{cases} 1 \;\; if \;\; \hat{y}_i^t \neq y_i \\ 0 \;\; if \;\; \hat{y}_i^t = y_i \end{cases}$$

   4.3 Compute the confidence α^t of the weak model t as

$$\alpha^t = \frac{1}{2}\Big(log\Big(\frac{1-\epsilon^t}{\epsilon^t}\Big)\Big)$$

   Note: In this formula, the confidence increases when the error decreases.

4.4 Update the weights as

- In a *regression* problem

$$w_i^{t+1} = \frac{w_i^t}{Z^t} \times \begin{cases} e^{\alpha^t} & if \ \ \frac{|\hat{y}_i^t - y_i|}{y_i} \geq threshold \\ e^{-\alpha^t} & if \ \ \frac{|\hat{y}_i^t - y_i|}{y_i} \leq threshold \end{cases} \quad for \quad i = 1, ..., N$$

  where Z^t is a normalization factor ensuring that $\sum_{i=1}^{N} w_i^{t+1} = 1$. *Note*: In this formula, the weight of each observation increases when the error increases.

- In a *classification* problem

$$w_i^{t+1} = \frac{w_i^t}{Z^t} \times \begin{cases} e^{\alpha^t} & if \ \ \hat{y}_i^t \neq y_i \\ e^{-\alpha^t} & if \ \ \hat{y}_i^t = y_i \end{cases} \quad for \quad i = 1, ..., N$$

  where Z^t is a normalization factor ensuring that $\sum_{i=1}^{N} w_i^{t+1} = 1$. *Note*: In this formula, the weight of each observation increases when the error increases.

5. Compute the single overall model ensembling the T models as

- In a *regression* problem

$$\hat{y}_i = \frac{\sum_{t=1}^{T} \alpha^t \hat{y}_i^t}{\sum_{t=1}^{T} \alpha^t} \quad for \quad i = 1, ..., N$$

  Note: The predictions of models with lower global error (higher confidence α^t) have more weight in the final prediction.

- In a *classification* problem with K categories in y

$$\hat{y}_i = max_k \left(\sum_{t=1}^{T} \alpha^t \times \begin{cases} 1 & if \ \ \hat{y}_i^t = k \\ 0 & if \ \ \hat{y}_i^t \neq k \end{cases} \right) \quad with \quad k = 1, ..., K \qquad for \quad i = 1, ..., N$$

  Note: The overall classification of each observation in the boosted final model is the class k more voted after aggregating the votes of the T models, giving more confidence to the models with a lower global error.

Thirdly, this paper covers the *AdaBoost* with *Classification Decision Tree (using Binary Splitting)* as the weak model in each iteration. Then, it is for *classification* problems and you can find all the necessary information about this model in the paper *Handmade_Decision_Tree.pdf*.

However, this model can be very complex if we build a *full tree*. It means that, if we do not set limitations when training, the tree grows until the *leaf nodes impurity* cannot be improved by a new split. Then, as we need a weak classifier in each *boosting* iteration, we will define the *maximum depth* of the tree as 2 (one split from the *root node* and one more split from each *son nodes*).

Note: We will use the implemented function *rpart* for *Decision Trees* in the R package *rpart*, setting all the parameters by default except of *maxdepth* equals to 2. It is appropriate because it includes the *weights* parameter, and we need it for the *boosting*.

CODE

The data used is the popular dataset *iris*. Let's predict the categorical variable *Species* (then it is a *classification* problem with 3 categories) with the explanatory features: *Sepal.Width* and *Petal.Width*.

Let's define the inputs x and y. Also, let's define x^{test} by creating artificial data with all combinations of both features from the minimum to the maximum values in x by 0.02, it will be interesting for observing the *AdaBoost decision boundaries* in the following plots.

```
x <- iris[,c("Sepal.Width","Petal.Width")]
y <- iris["Species"]
x_test <- expand.grid(list(Sepal.Width=seq(min(x[,1]),max(x[,1]),0.02),
                           Petal.Width=seq(min(x[,2]),max(x[,2]),0.02)))
```

Let's create the *weak_model* function which uses the inputs x and y for training a *Classification Decision Tree*, with *maxdepth* 2 and determined *weights*, and also computes the predictions for the input x^{test}.

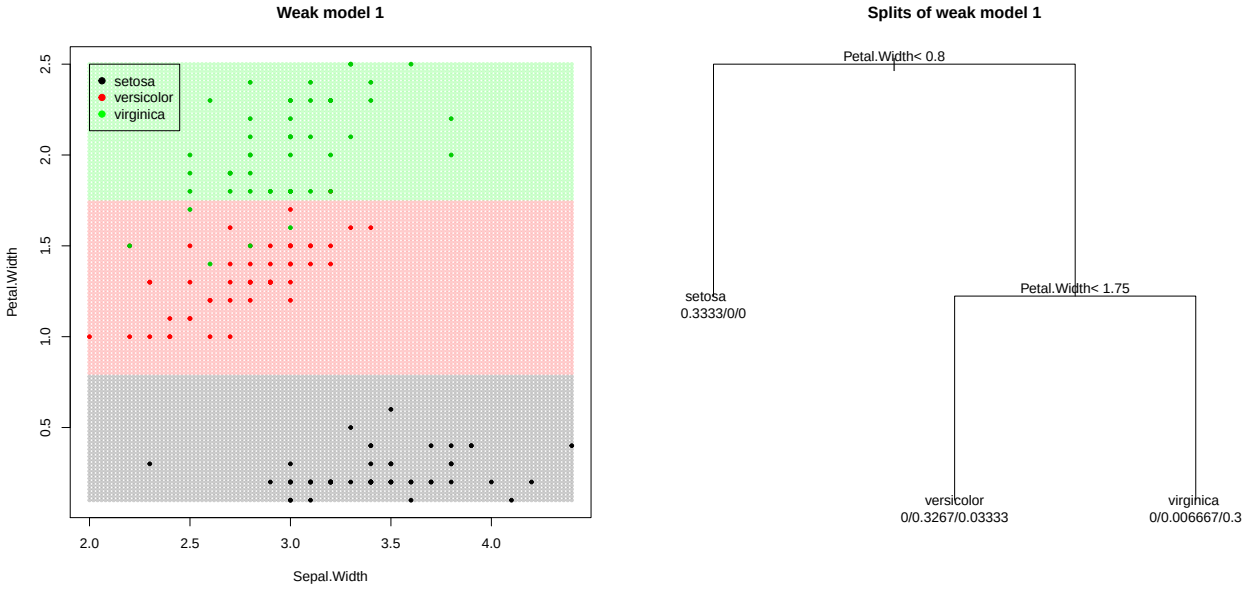
```
weak_model <- function(x,y,x_test,weights){
  library(rpart)
  decision_tree <- rpart(y~Sepal.Width+Petal.Width,data=x,method="class",weights=weights,
                         control=rpart.control(maxdepth=2))
  predictions <- predict(object=decision_tree,newdata=x_test,type="class")
  return(list(decision_tree=decision_tree,predictions=predictions))
}
```

Let's create the *AdaBoost* algorithm.

```
AdaBoost <- function(x,y,x_test,weak_model,iterations){
  N <- nrow(x)
  K <- length(unique(y))
  N_test <- nrow(x_test)
  predictions <- rep(0,times=N)
  error <- rep(0,times=iterations)
  confidence <- rep(0,times=iterations)
  # Create a matrix for the single overall model prediction of x_test
  predictions_test <- matrix(0,nrow=N_test,ncol=K)
  # Initiliaze the weights uniformly
  weights <- rep(1/N,times=N)
  # Iterate the T boosting iterations
  for(t in 1:iterations){
    # Train the weak model t and compute the predictions for x and x_test
    predictions_t <- weak_model(x,y,x,weights)$predictions
    predictions_test_t <- weak_model(x,y,x_test,weights)$predictions
    # Compute the global error of the weak model t
    error[t] <- sum(weights*(predictions_t!=y))
    # Compute the confidence of the weak model t
    confidence[t] <- 1/2*log((1-error[t])/error[t])
    # Update the weight
    weights <- weights*exp(confidence[t]*(-1)^(predictions_t==y))
    weights <- weights/sum(weights)
    # For each x_test observation, sum the weak model t confidence to the predicted class
    for(i in 1:N_test){
      k <- predictions_test_t[i]
      predictions_test[i,k] <- predictions_test[i,k] + confidence[t]
    }
  }
  # Compute the single overall model prediction for x_test
  y_test <- rep(0,times=N_test)
  for(i in 1:N_test){
      y_test[i] <- which.max(predictions_test[i,])
  }
  return(y_test)
}
```

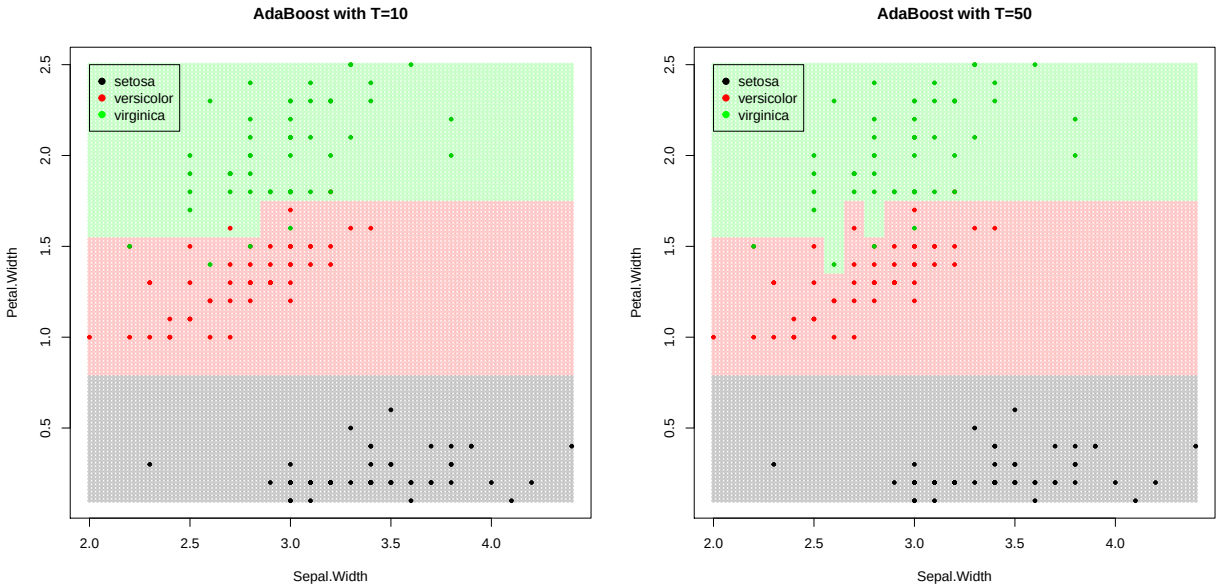
Now, let's apply the first weak model (iteration 1 of *boosting* with uniform weights) and plot the result.

```
par(mfrow=c(1,2),xpd=TRUE)
# Train the weak model 1
weak_model_1 <- weak_model(x,y,x_test,weights=rep(1/nrow(x),times=nrow(x)))
# Decision boundaries
predictions <- weak_model_1$predictions
transparent_colors <- scales::alpha(c("black","red","green"),0.2)
plot(x_test[,1],x_test[,2],col=transparent_colors[as.numeric(predictions)],
     pch=19,cex=0.5,xlab="Sepal.Width",ylab="Petal.Width",main="Weak model 1")
points(x[,1],x[,2],col=y,pch=19,cex=0.6)
legend(2,2.5,legend=unique(y),col=c("black","red","green"),pch=19)
# Splits
plot(weak_model_1$decision_tree,main="Splits of weak model 1")
text(weak_model_1$decision_tree,use.n=TRUE)
```



Now, let's apply the *AdaBoost* with 10 and 50 iterations, and plot the result.

```
par(mfrow=c(1,2))
# AdaBoost with 10 iterations
predictions <- AdaBoost(x,y,x_test,weak_model,10)
transparent_colors <- scales::alpha(c("black","red","green"),0.2)
plot(x_test[,1],x_test[,2],col=transparent_colors[as.numeric(predictions)],
     pch=19,cex=0.5,xlab="Sepal.Width",ylab="Petal.Width",main="AdaBoost with T=10")
points(x[,1],x[,2],col=y,pch=19,cex=0.6)
legend(2,2.5,legend=unique(y),col=c("black","red","green"),pch=19)
# AdaBoost with 50 iterations
predictions <- AdaBoost(x,y,x_test,weak_model,50)
transparent_colors <- scales::alpha(c("black","red","green"),0.2)
plot(x_test[,1],x_test[,2],col=transparent_colors[as.numeric(predictions)],
     pch=19,cex=0.5,xlab="Sepal.Width",ylab="Petal.Width",main="AdaBoost with T=50")
points(x[,1],x[,2],col=y,pch=19,cex=0.6)
legend(2,2.5,legend=unique(y),col=c("black","red","green"),pch=19)
```



In conclusion, in this plots, we can observe the predictions for x^{test} (transparent coloured points) and the real values y (solid coloured points). Also, we can observe the *decision boundary* for each class in the target variable *Species* in the *iris* data.

Comparing the plots of three models (first weak model and two versions of *AdaBoost*), the decision boundaries are more complex and smooth when increasing the number of *boosting* iterations and this is because each iteration improves the previous predictions. Then, the more iterations, the more chances to classify well the misclassified observations.

Note: Remember that we are using always the same weak model (*Classification Decision Tree* with *maxdepth* 2) and we get smoother decision boundaries and higher accuracy in the single overall model just *boosting* it. It is really useful because it enables us to improve our model without changing it for another more complex.