Handmade AdaBoost

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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.

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 $w^t_{[Nx1]}$, and the inputs $x_{[NxP]}$ and $y_{[Nx1]}$. Then, compute the predictions $\hat{y}^t_{[Nx1]}$.

   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^{target} 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_target <- 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^{target}.

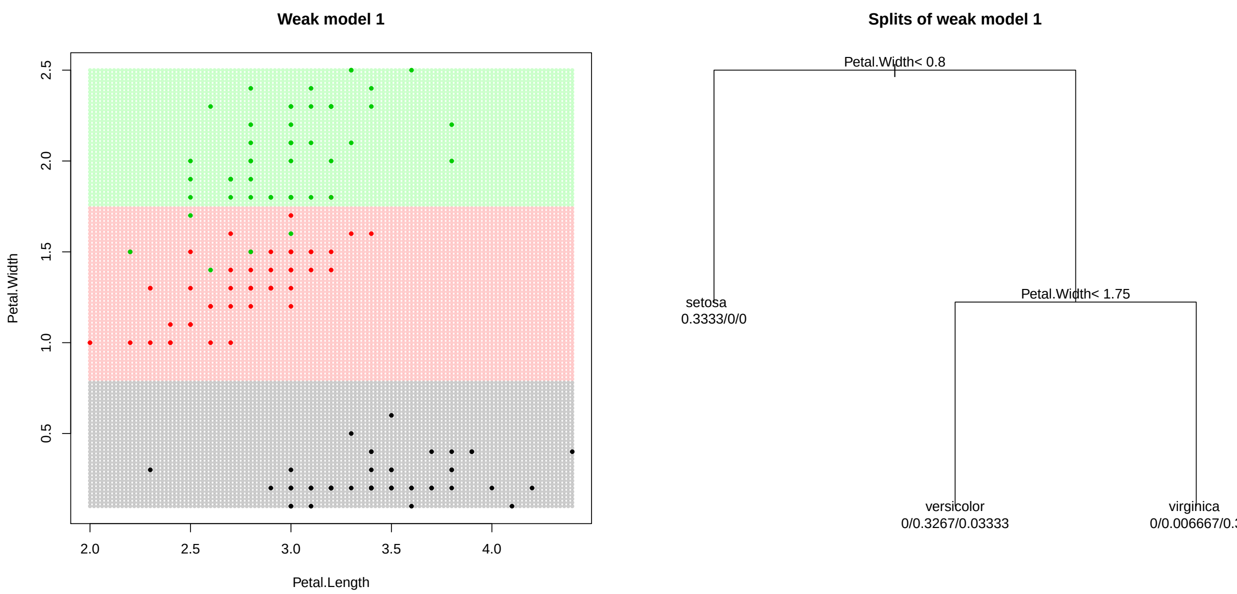
```
weak_model <- function(x,y,x_target,weights){
  library(rpart)
  decision_tree <- rpart(y~Sepal.Width+Petal.Width,data=x,method="class",weights=weights,
                         control=rpart.control(maxdepth=2))
  predictions <- predict(object=decision_tree,newdata=x_target,type="class")
  return(list(decision_tree=decision_tree,predictions=predictions))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

Let's create the *AdaBoost* algorithm.

```
AdaBoost <- function(x,y,x_target,weak_model,iterations){
  N <- nrow(x)
  K <- length(unique(y))
  N_target <- nrow(x_target)
  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_target
  predictions_target <- matrix(0,nrow=N_target,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_target
    predictions_t <- weak_model(x,y,x,weights)$predictions
    predictions_target_t <- weak_model(x,y,x_target,weights)$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_target observation, sum the weak model t confidence to the predicted class
    for(i in 1:N_target){
      k <- predictions_target_t[i]
      predictions_target[i,k] <- predictions_target[i,k] + confidence[t]
    }
  }
  # Compute the single overall model prediction for x_target
  y_target <- rep(0,times=N_target)
  for(i in 1:N_target){
      y_target[i] <- which.max(predictions_target[i,])
  }
  return(y_target)
}
```

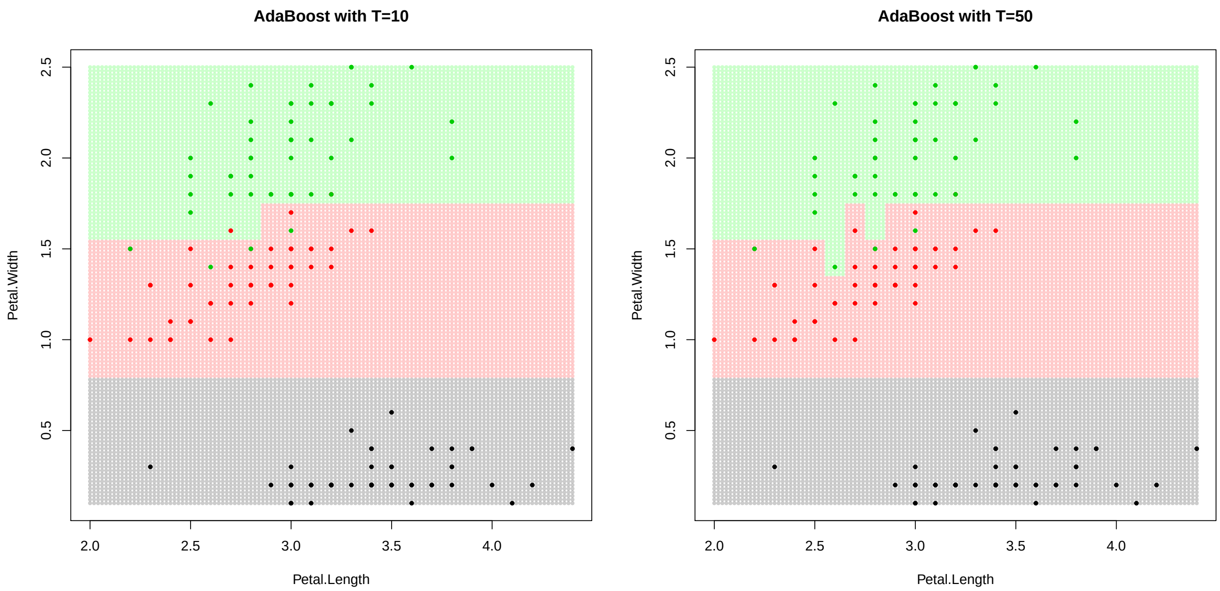
Now, let's apply the first weak model (iteration 1 of *boosting* with uniform weights) and plot the result.

```
par(mfrow=c(1,2),xpd=TRUE)
# Train the weak model 1
weak_model_1 <- weak_model(x,y,x_target,weights=rep(1/nrow(x),times=nrow(x)))
# Decision boundaries
predictions <- weak_model_1$predictions
transparent_colors <- scales::alpha(c("black","red","green"),0.2)
plot(x_target[,1],x_target[,2],col=transparent_colors[as.numeric(predictions)],
     pch=19,cex=0.5,xlab="Petal.Length",ylab="Petal.Width",main="Weak model 1")
points(x[,1],x[,2],col=y,pch=19,cex=0.6)
legend(1,1.5,legend=unique(y),col=c("black","red","green"),pch=19,cex=0.7)
# Splits
plot(weak_model_1$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_target,weak_model,10)
transparent_colors <- scales::alpha(c("black","red","green"),0.2)
plot(x_target[,1],x_target[,2],col=transparent_colors[as.numeric(predictions)],
     pch=19,cex=0.5,xlab="Petal.Length",ylab="Petal.Width",main="AdaBoost with T=10")
points(x[,1],x[,2],col=y,pch=19,cex=0.6)
legend(1,1.5,legend=unique(y),col=c("black","red","green"),pch=19,cex=0.7)
# AdaBoost with 50 iterations
predictions <- AdaBoost(x,y,x_target,weak_model,50)
transparent_colors <- scales::alpha(c("black","red","green"),0.2)
plot(x_target[,1],x_target[,2],col=transparent_colors[as.numeric(predictions)],
     pch=19,cex=0.5,xlab="Petal.Length",ylab="Petal.Width",main="AdaBoost with T=50")
points(x[,1],x[,2],col=y,pch=19,cex=0.6)
legend(1,1.5,legend=unique(y),col=c("black","red","green"),pch=19,cex=0.7)
```



In conclusion, in this plots, we can observe the predictions for x^{target} (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.