Ensemble Methods

Adaptive and Gradient Boosting

Santander Meteorology Group

Objetivo:

En la presente práctica trataremos de profundizar en la utilización de los métodos de basados ensembles y compararlos con su contrapartida basada en árboles. Para ello, en primer lugar instalaremos los paquetes asociados a los métodos de ensembles

```
install.packages("randomForest")
install.packages("adabag")
install.packages("gbm")
```

y cargamos las librerías correspondientes:

```
library(tree) ## arboles

library(rpart) ## Tree-based model

library(randomForest) ## bagging: random forests

library(adabag) ## boosting: adaptive boosting

library(gbm) ## boosting: Gradient boosting

library(caret)

library(MASS)
```

A lo largo de la práctica usaremos varios datasets para ejemplificar el uso de las diferentes funciones.

Clasificación:

Ejemplo: Iris dataset

Cargamos los datos y definimos los conjuntos de train y de test:

```
## train/test partition
set.seed(23)
n <- nrow(iris)
indtrain <- sample(1:n, round(0.75*n)) # indices for train
indtest <- setdiff(1:n, indtrain) # indices for test</pre>
```

y predecimos y evaluamos sobre ambos conjuntos utilizando un árbol de decisión:

[1] 0.9210526 1.0000000

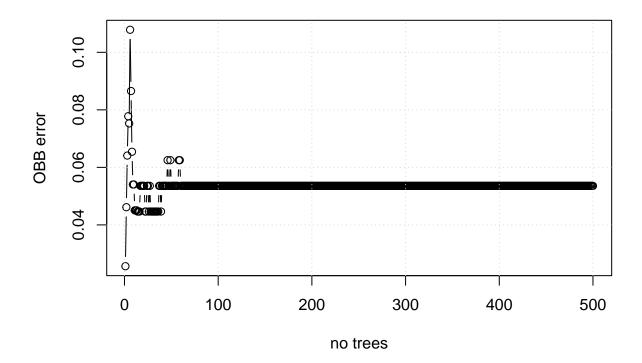
A continuación, siguiendo con lo visto en la sesión anterior, realizamos la predicción considerando los random forest utilizando el valor por defector para el número de variables seleccionadas para cada árbol:

```
set.seed(23)
## Bagging: Random Forests

rf <- randomForest(Species ~., iris , subset = indtrain, ntree = 500, mtry = 2)

# OOB error

plot(rf$err.rate[, 1], type = "b", xlab = "no trees",
ylab = "OBB error")
grid()</pre>
```



A la vista de los resultados consideramos el número de árboles óptimo sobre 100 dado que es la zona de estabilización del parámetros de validación:

[1] 0.9473684 1.0000000

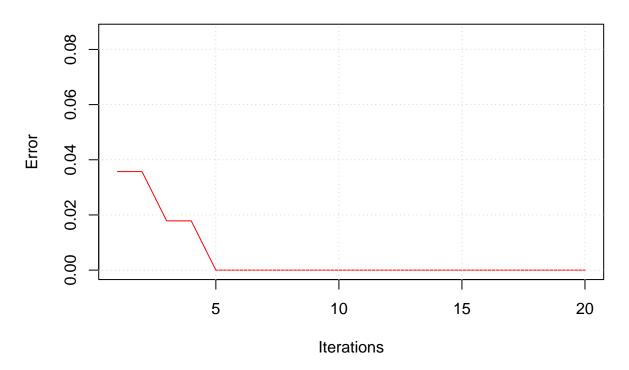
Consideremos ahora el método estándar de boosting, el Adaptive Boosting (adaboost). Para ello, revisemos inicialmente los parámetros de la función boosting:

```
## Boosting: Adaptive Boosting (AdaBoost)
? boosting
```

Dado el tamaño del dataset, consideremos un número limitado de árboles, pero suficientemente grande, para ver el número óptimo de árboles a utilizar:

```
# AdaBoost with 20 trees (mfinal)
ab = boosting(Species ~., iris[indtrain, ], mfinal = 20, boos = FALSE)
# train errors as a function of number of trees
plot(errorevol(ab, iris[indtrain, ]))
grid()
```

Ensemble error vs number of trees



Como vemos, a partir de 5 árboles ya el error es nulo, de modo que el número máximo de árboles debe ser a lo sumo 5.

```
## Boosting: Adaptive Boosting (AdaBoost)
## 20 trees (mfinal)
ab <- boosting(Species ~., iris[indtrain, ], mfinal = 5)
## Prediction for test
pred.ab.test <- predict(ab, iris[indtest, ])
## Prediction for train
pred.ab.train <- predict(ab, iris[indtrain, ])
## Accuracy
c(sum(diag(table(pred.ab.test$class, iris$Species[indtest]))) / length(indtest),
    sum(diag(table(pred.ab.train$class, iris$Species[indtrain]))) / length(indtrain))</pre>
```

[1] 0.9210526 0.9910714

Al considerar árboles, y como dice la ayuda, podemos definir los parámetros de control de los árboles construidos con la función rpart:

[1] 0.9473684 1.0000000

Finalmente, consideremos el Gradient Boosting para lo cual revisemos los parámetros de la función gbm:

? gbm

Los argumentos base vistos en la sesión teórica se corresponden con:

- shrinkage
- n.trees
- interaction.depth

Si bien hay otros argumentos que permiten el control de las caracteristicas de los arboles, la validación cruzada o la aleatorización del conjunto de entrenamiento.

Distribution not specified, assuming multinomial ...

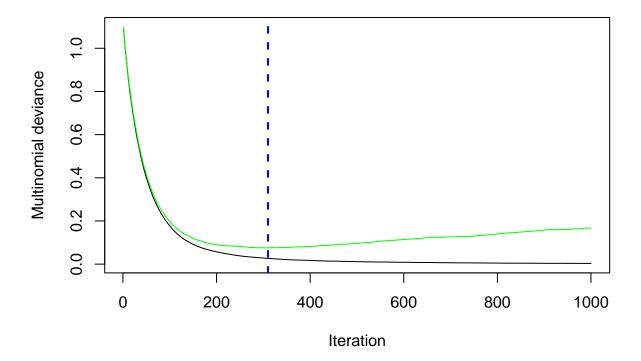
¿Cuántos árboles seleccionarías?

```
## [1] 0.9210526 1.0000000
```

Como dijimos, pueden incluirse parámetros que controlen la validación cruzada, obteniendo el valor óptimo:

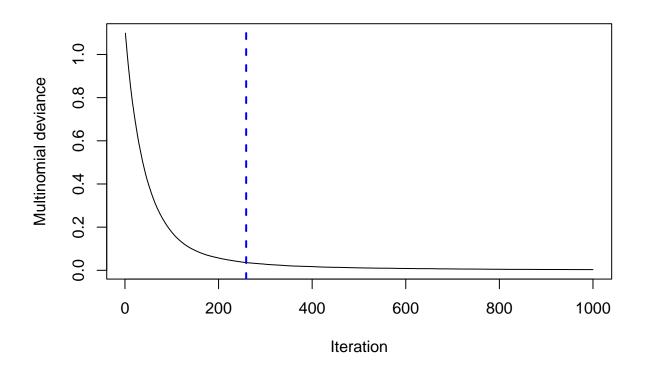
Distribution not specified, assuming multinomial ...

```
ntree_opt_cv <- gbm.perf(gb.cv, method = "cv")</pre>
```



```
ntree_opt_oob <- gbm.perf(gb.cv, method = "OOB")</pre>
```

00B generally underestimates the optimal number of iterations although predictive performance



```
print(ntree_opt_cv)

## [1] 310

print(ntree_opt_oob)

## [1] 259

## attr(,"smoother")

## Call:

## loess(formula = object$oobag.improve ~ x, enp.target = min(max(4, ## length(x)/10), 50))

##

## Number of Observations: 1000

## Equivalent Number of Parameters: 40

## Residual Standard Error: 0.0005396
```

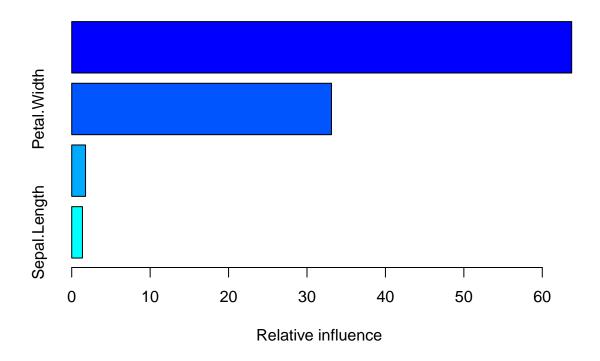
Que podemos usar en el ajuste:

Distribution not specified, assuming multinomial ...

```
print(gb)
```

```
## gbm(formula = Species ~ ., data = iris[indtrain, ], n.trees = ntree_opt_cv,
## interaction.depth = 20, shrinkage = 0.01)
## A gradient boosted model with multinomial loss function.
## 310 iterations were performed.
## There were 4 predictors of which 4 had non-zero influence.
```

summary(gb)



var rel.inf
Petal.Length Petal.Length 63.748011

[1] 0.9210526 1.0000000

Petal.Width

Petal.Width 33.121518

Nuevas implementaciones optimizan el algoritmo realizando el ajuste de forma más eficiente, las cuales probaremos con el dataset Meteo:

```
install.packages("xgboost") ## Extreme Gradient Boosting
```

Ejemplo: Meteo dataset

```
library(MASS)
library(tree)
library(randomForest)
library(adabag)
library(gbm)
library(caret)
library(xgboost)
```

Cargamos los datos

```
load("~/meteo.RData")
```

y definimos los conjuntos de train y de test:

```
## Keeping the first 10 years (3650 days) for this example
n <- 3650
y <- y[1:n]
x <- x[1:n, ]
## train/test partition
set.seed(23)
indtrain <- sample(1:n, round(0.75*n)) # indices for train
indtest <- setdiff(1:n, indtrain) # indices for test</pre>
```

Sigamos con el caso de clasificación:

```
## binary occurrence (1/0)
occ <- y
occ[which(y < 1)] <- 0
occ[which(y >= 1)] <- 1
## dataframe for occurrence
df.occ <- data.frame(y.occ = as.factor(occ), predictors = x)</pre>
```

y probemos las diferentes técnicas vistas a lo largo del curso.

Decision Trees:

```
print(c(sum(diag(table(pred.t.test, df.occ$y.occ[indtest]))) / length(indtest),
        sum(diag(table(pred.t.train, df.occ$y.occ[indtrain]))) / length(indtrain)))
## [1] 0.8267544 1.0000000
Para discutir más en profundidad la validación obtengamos las matrices de confusión para el test
confusionMatrix(pred.t.test, df.occ$y.occ[indtest])
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction
                0
                    1
            0 649
##
                   73
            1 85 105
##
##
##
                  Accuracy : 0.8268
##
                    95% CI: (0.8006, 0.8508)
       No Information Rate: 0.8048
##
       P-Value [Acc > NIR] : 0.05007
##
##
##
                     Kappa : 0.4623
##
    Mcnemar's Test P-Value: 0.38151
##
##
               Sensitivity: 0.8842
##
               Specificity: 0.5899
##
            Pos Pred Value: 0.8989
##
            Neg Pred Value: 0.5526
                Prevalence: 0.8048
##
##
            Detection Rate: 0.7116
```

##

Detection Prevalence: 0.7917

```
##
         Balanced Accuracy: 0.7370
##
          'Positive' Class : 0
##
##
y el train:
confusionMatrix(pred.t.train, df.occ$y.occ[indtrain])
## Confusion Matrix and Statistics
##
             Reference
##
## Prediction
                 0
            0 2171
##
##
                 0 567
##
                  Accuracy : 1
##
                    95% CI: (0.9987, 1)
##
       No Information Rate: 0.7929
##
       P-Value [Acc > NIR] : < 2.2e-16
##
##
##
                     Kappa: 1
##
   Mcnemar's Test P-Value : NA
##
##
               Sensitivity: 1.0000
               Specificity: 1.0000
##
##
            Pos Pred Value : 1.0000
##
            Neg Pred Value : 1.0000
                Prevalence: 0.7929
##
##
            Detection Rate: 0.7929
```

Detection Prevalence: 0.7929

##

```
##
         Balanced Accuracy: 1.0000
##
          'Positive' Class : 0
##
##
Bagging: Random Forests
## Single Tree:
rf <- randomForest(y.occ ~., df.occ, subset = indtrain, ntree = 500)</pre>
## Prediction for test
pred.rf.test <- predict(rf, df.occ[indtest, ])</pre>
## Prediction for train
pred.rf.train <- predict(rf, df.occ[indtrain, ])</pre>
## Accuracy
print(c(sum(diag(table(pred.rf.test, df.occ$y.occ[indtest]))) / length(indtest),
        sum(diag(table(pred.rf.train, df.occ$y.occ[indtrain]))) / length(indtrain)))
## [1] 0.8804825 1.0000000
Para discutir más en profundidad la validación obtengamos las matrices de confusión para el test
confusionMatrix(pred.rf.test, df.occ$y.occ[indtest])
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction
            0 696 71
##
##
            1 38 107
##
##
                  Accuracy : 0.8805
                     95% CI: (0.8576, 0.9008)
##
```

##

No Information Rate: 0.8048

```
P-Value [Acc > NIR] : 6.949e-10
##
##
##
                     Kappa: 0.5908
##
   Mcnemar's Test P-Value: 0.002176
##
##
               Sensitivity: 0.9482
##
               Specificity: 0.6011
##
            Pos Pred Value: 0.9074
##
            Neg Pred Value: 0.7379
##
                Prevalence: 0.8048
##
##
            Detection Rate: 0.7632
##
      Detection Prevalence: 0.8410
##
         Balanced Accuracy: 0.7747
##
          'Positive' Class : 0
##
##
y el train:
confusionMatrix(pred.rf.train, df.occ$y.occ[indtrain])
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction
                 0
            0 2171
                      0
##
##
            1
                 0 567
##
                  Accuracy : 1
##
##
                    95% CI : (0.9987, 1)
##
       No Information Rate: 0.7929
```

```
##
       P-Value [Acc > NIR] : < 2.2e-16
##
                     Kappa: 1
##
##
   Mcnemar's Test P-Value : NA
##
##
##
               Sensitivity: 1.0000
               Specificity: 1.0000
##
            Pos Pred Value : 1.0000
##
            Neg Pred Value: 1.0000
##
                Prevalence: 0.7929
##
            Detection Rate: 0.7929
##
      Detection Prevalence: 0.7929
##
##
         Balanced Accuracy: 1.0000
##
##
          'Positive' Class : 0
##
```

Boosting: Adaptive Boosting (AdaBoost)

[1] 0.8684211 1.0000000

Para discutir más en profundidad la validación obtengamos las matrices de confusión para el test

```
confusionMatrix(as.factor(pred.ab.test$class), df.occ$y.occ[indtest])
```

```
## Confusion Matrix and Statistics
##
             Reference
##
## Prediction
                0
##
            0 681 67
##
            1 53 111
##
                  Accuracy : 0.8684
##
                    95% CI: (0.8447, 0.8897)
##
       No Information Rate: 0.8048
##
##
       P-Value [Acc > NIR] : 2.486e-07
##
##
                     Kappa : 0.5683
##
   Mcnemar's Test P-Value: 0.2353
##
##
##
               Sensitivity: 0.9278
               Specificity: 0.6236
##
##
            Pos Pred Value: 0.9104
##
            Neg Pred Value: 0.6768
##
                Prevalence: 0.8048
            Detection Rate: 0.7467
##
##
      Detection Prevalence: 0.8202
##
         Balanced Accuracy: 0.7757
##
##
          'Positive' Class : 0
##
```

y el train:

##

```
## Confusion Matrix and Statistics
##
             Reference
##
## Prediction
                 0
##
            0 2171
                      0
##
            1
                 0 567
##
                  Accuracy : 1
##
                    95% CI : (0.9987, 1)
##
       No Information Rate: 0.7929
##
##
       P-Value [Acc > NIR] : < 2.2e-16
##
                     Kappa: 1
##
##
   Mcnemar's Test P-Value : NA
##
##
##
               Sensitivity: 1.0000
##
               Specificity: 1.0000
##
            Pos Pred Value : 1.0000
##
            Neg Pred Value : 1.0000
##
                Prevalence: 0.7929
            Detection Rate: 0.7929
##
##
      Detection Prevalence: 0.7929
##
         Balanced Accuracy : 1.0000
##
##
          'Positive' Class : 0
```

confusionMatrix(as.factor(pred.ab.train\$class), df.occ\$y.occ[indtrain])

Boosting: eXtreme Gradient Boosting

```
df.gb.occ <- df.occ</pre>
df.gb.occ$y.occ <- as.character(df.gb.occ$y.occ)</pre>
gb <- xgboost(data = x[indtrain,], label = df.gb.occ$y.occ[indtrain], max.depth = 6, eta = 1, nr
               nthread = 2, objective = "binary:logistic")
## [14:22:39] WARNING: amalgamation/../src/learner.cc:1115: Starting in XGBoost 1.3.0, the defau
## [1] train-logloss:0.268630
print(gb)
## #### xgb.Booster
## raw: 8.2 Kb
## call:
     xgb.train(params = params, data = dtrain, nrounds = nrounds,
##
##
       watchlist = watchlist, verbose = verbose, print every n = print every n,
##
       early_stopping_rounds = early_stopping_rounds, maximize = maximize,
##
       save_period = save_period, save_name = save_name, xgb_model = xgb_model,
##
       callbacks = callbacks, max.depth = 6, eta = 1, nthread = 2,
       objective = "binary:logistic")
##
## params (as set within xgb.train):
     max_depth = "6", eta = "1", nthread = "2", objective = "binary:logistic", validate_paramete
##
## xgb.attributes:
##
     niter
## callbacks:
     cb.print.evaluation(period = print_every_n)
##
##
     cb.evaluation.log()
## niter: 1
## nfeatures : 320
## evaluation_log:
```

```
0.26863
##
summary(gb)
                                             Mode
##
                  Length Class
## handle
                          xgb.Booster.handle externalptr
                  8309
## raw
                          -none-
                                             raw
## niter
                      1
                          -none-
                                             numeric
## evaluation_log
                          data.table
                                             list
## call
                     17
                          -none-
                                              call
## params
                     5
                          -none-
                                             list
## callbacks
                     2
                          -none-
                                             list
## nfeatures
                      1
                          -none-
                                             numeric
## Prediction for test
pred.gb.test <- predict(gb, newdata = x[indtest, ], type = "response")</pre>
## Prediction for train
pred.gb.train <- predict(gb, newdata = x[indtrain, ], type = "response")</pre>
## Accuracy
pred.gb.test.bin <- as.factor(ifelse(pred.gb.test>mean(as.numeric(df.gb.occ\$y.occ[indtrain])),1
pred.gb.train.bin <- as.factor(ifelse(pred.gb.train>mean(as.numeric(df.gb.occ$y.occ[indtrain]))
print(c(sum(diag(table(pred.gb.test.bin, df.gb.occ$y.occ[indtest]))) / length(indtest),
        sum(diag(table(pred.gb.train.bin, df.gb.occ$y.occ[indtrain]))) / length(indtrain)))
## [1] 0.8223684 0.8703433
Para discutir más en profundidad la validación obtengamos las matrices de confusión para el test
confusionMatrix(pred.gb.test.bin, df.occ$y.occ[indtest])
## Confusion Matrix and Statistics
##
```

iter train_logloss

```
Reference
##
              0
## Prediction
            0 618 46
##
           1 116 132
##
##
##
                  Accuracy : 0.8224
                    95% CI: (0.796, 0.8466)
##
       No Information Rate: 0.8048
##
       P-Value [Acc > NIR] : 0.0966
##
##
                     Kappa : 0.5079
##
##
##
   Mcnemar's Test P-Value : 5.922e-08
##
               Sensitivity: 0.8420
##
               Specificity: 0.7416
##
            Pos Pred Value: 0.9307
##
            Neg Pred Value: 0.5323
##
##
                Prevalence: 0.8048
##
            Detection Rate: 0.6776
      Detection Prevalence : 0.7281
##
##
         Balanced Accuracy: 0.7918
##
##
          'Positive' Class : 0
##
y el train:
confusionMatrix(pred.gb.train.bin, df.occ$y.occ[indtrain])
## Confusion Matrix and Statistics
##
```

```
##
             Reference
## Prediction
            0 1884
                     68
##
            1 287
                    499
##
##
##
                  Accuracy : 0.8703
                    95% CI: (0.8572, 0.8827)
##
       No Information Rate: 0.7929
##
       P-Value [Acc > NIR] : < 2.2e-16
##
##
                     Kappa : 0.6545
##
##
##
    Mcnemar's Test P-Value : < 2.2e-16
##
               Sensitivity: 0.8678
##
               Specificity: 0.8801
##
            Pos Pred Value: 0.9652
##
            Neg Pred Value: 0.6349
##
##
                Prevalence: 0.7929
            Detection Rate: 0.6881
##
      Detection Prevalence: 0.7129
##
         Balanced Accuracy: 0.8739
##
##
          'Positive' Class : 0
##
##
```

Predicción:

A modo de ejemplo hemos utilizado el dataset Boston para problemas de predicción.

```
library(MASS)

n <- nrow(Boston)
# train/test partition
indtrain <- sample(1:n, round(0.75*n)) # indices for train
indtest <- setdiff(1:n, indtrain) # indices for test

# RF

rf <- randomForest(medv ~., Boston , subset = indtrain)
# RF configuration?

# 00B error?
plot(rf$mse, type = "l", xlab = "no. trees", ylab = "00B error")
grid()</pre>
```

Extender el análisis hecho para el problema de clasificación a este dataset, comparando las diferentes aproximaciones.

Session Info:

```
[5] LC MONETARY=es ES.UTF-8
                                   LC MESSAGES=en US.UTF-8
##
    [7] LC PAPER=es ES.UTF-8
##
                                   LC NAME=C
    [9] LC ADDRESS=C
##
                                   LC TELEPHONE=C
## [11] LC MEASUREMENT=es ES.UTF-8 LC IDENTIFICATION=C
##
## attached base packages:
## [1] parallel stats
                           graphics grDevices utils
                                                          datasets methods
## [8] base
##
## other attached packages:
    [1] xgboost 1.5.0.2
                            MASS 7.3-54
                                                gbm 2.1.8
   [4] adabag 4.2
                            doParallel 1.0.16
                                                 iterators 1.0.13
   [7] foreach_1.5.1
                            caret_6.0-90
                                                 lattice 0.20-45
##
## [10] ggplot2 3.3.5
                            randomForest 4.6-14 rpart 4.1-15
## [13] tree 1.0-41
##
## loaded via a namespace (and not attached):
    [1] Rcpp_1.0.6
                             lubridate 1.8.0
                                                   listenv 0.8.0
   [4] class_7.3-19
                             digest 0.6.27
                                                   ipred 0.9-12
##
##
  [7] utf8_1.2.2
                             parallelly_1.29.0
                                                   R6_2.5.0
## [10] plyr_1.8.6
                             stats4_4.1.2
                                                   e1071_1.7-9
## [13] evaluate 0.14
                             highr 0.8
                                                   pillar 1.6.4
                                                   Matrix_1.4-0
## [16] rlang_0.4.12
                             data.table_1.14.2
## [19] rmarkdown_2.11
                             splines_4.1.2
                                                   gower_0.2.2
## [22] stringr_1.4.0
                             munsell_0.5.0
                                                   proxy_0.4-26
## [25] compiler 4.1.2
                             xfun 0.29
                                                   pkgconfig_2.0.3
## [28] globals_0.14.0
                             htmltools_0.5.1.1
                                                   nnet 7.3-16
## [31] tidyselect_1.1.1
                             tibble_3.1.6
                                                   prodlim_2019.11.13
## [34] codetools_0.2-18
                             fansi_0.5.0
                                                   future_1.23.0
## [37] crayon_1.4.2
                             dplyr 1.0.7
                                                   withr 2.4.3
```

## [40] recipes_0.1.17	ModelMetrics_1.2.2.2	2 grid_4.1.2
## [43] jsonlite_1.7.2	nlme_3.1-152	gtable_0.3.0
## [46] lifecycle_1.0.1	magrittr_2.0.1	pROC_1.18.0
## [49] scales_1.1.1	future.apply_1.8.1	stringi_1.5.3
## [52] reshape2_1.4.4	timeDate_3043.102	ellipsis_0.3.2
## [55] generics_0.1.1	vctrs_0.3.8	lava_1.6.10
## [58] tools_4.1.2	glue_1.4.2	purrr_0.3.4
## [61] survival_3.2-13	yaml_2.2.1	colorspace_2.0-2
## [64] knitr_1.31		