Ensembles Lab 2: Boosting

Adapted by EVL, FRC and ASP

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```r
# Helper packages
library(dplyr)       # for data wrangling
library(ggplot2)     # for awesome plotting
library(modeldata)
library(foreach)     # for parallel processing with for loops

# Modeling packages
# library(tidymodels)
library(xgboost)
library(gbm)
```

Introduction

This lab continues on the previous one showing how to apply boosting. The same dataset as before will be used

Ames Housing dataset

Packge `AmesHousing` contains the data jointly with some instructions to create the required dataset.

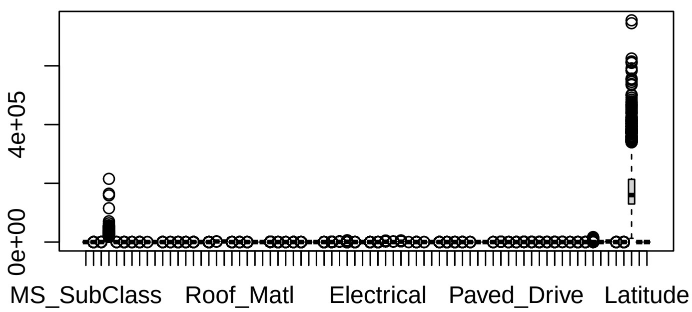
We will use, however data from the `modeldata` package where some preprocessing of the data has already been performed (see: https://www.tmwr.org/ames)

The dataset has 74 variables so a descriptive analysis is not provided.

```r
dim(ames)
```

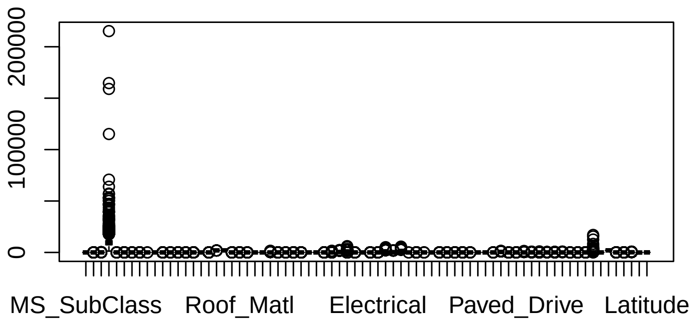
```
[1] 2930   74
```

```r
boxplot(ames)
```



We proceed as in the previous lab and divide the reponse variable by 1000 facilitate reviewing the results .

```r
require(dplyr)
ames <- ames %>% mutate(Sale_Price = Sale_Price/1000)
boxplot(ames)
```



Spliting the data into test/train

The data are split in separate test / training sets and do it in such a way that samplig is balanced for the response variable, `Sale_Price`.

```
# Stratified sampling with the rsample package
set.seed(123)
split <- rsample::initial_split(ames, prop = 0.7,
                                strata = "Sale_Price")
ames_train  <- training(split)
ames_test   <- testing(split)
```

Parameter optimization

Tree number

This is a critical parameter as far as adding new trees increases risk of overfitting.

Before optimization is run, data is shaped into an object of class `xgb.DMatrix`, which is required to run XGBoost through this package.

```r
ames_train_num <- model.matrix(Sale_Price ~ . , data = ames_train)[,-1]
ames_test_num <- model.matrix(Sale_Price ~ . , data = ames_test)[,-1]

train_labels <- ames_train$Sale_Price
test_labels <- ames_test$Sale_Price

ames_train_matrix <- xgb.DMatrix(
  data = ames_train_num,
  label = train_labels
)

ames_test_matrix <- xgb.DMatrix(
  data = ames_test_num,
  label = test_labels
)
```

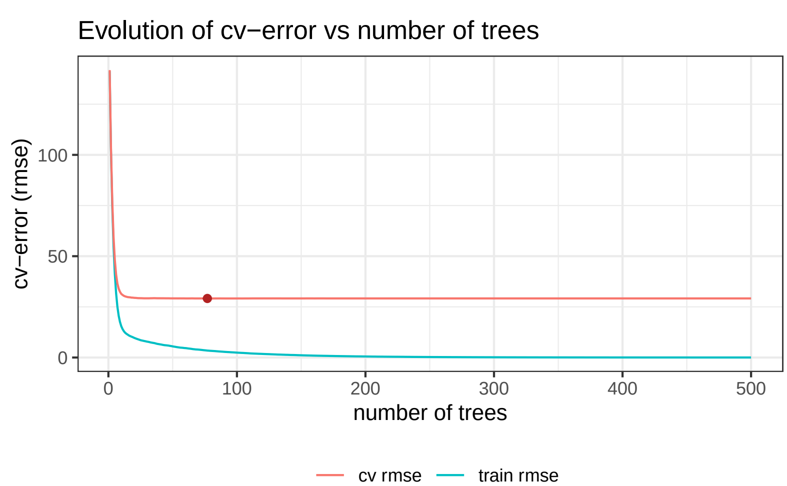
```r
boostResult_cv <- xgb.cv(
  data = ames_train_matrix,
  params = list(eta = 0.3, max_depth = 6, subsample = 1, objective = "reg:squarederror"),
  nrounds = 500,
  nfold = 5,
  metrics = "rmse",
  verbose = 0
)

boostResult_cv <- boostResult_cv$evaluation_log
print(boostResult_cv)
```

```
      iter train_rmse_mean train_rmse_std test_rmse_mean test_rmse_std
     <num>           <num>          <num>          <num>         <num>
  1:     1    1.412915e+02   0.9570592195      141.81926      3.756892
  2:     2    1.019455e+02   0.7941089688      103.61188      3.395008
  3:     3    7.430242e+01   0.7320607454       77.11700      3.556748
  4:     4    5.479365e+01   0.6093311366       59.41119      3.735165
  5:     5    4.118576e+01   0.5362387078       48.04453      4.272442
 ---
496:   496    7.383272e-03   0.0006022381       29.16183      4.817437
497:   497    7.293321e-03   0.0005722715       29.16184      4.817432
498:   498    7.164931e-03   0.0005468412       29.16184      4.817431
499:   499    7.053888e-03   0.0005474267       29.16184      4.817429
```

```
500:    500     6.977090e-03    0.0005256163        29.16187      4.817472
```

We aim at at the lowest number of trees that has associated a small cross-validation error.

```r
ggplot(data = boostResult_cv) +
  geom_line(aes(x = iter, y = train_rmse_mean, color = "train rmse")) +
  geom_line(aes(x = iter, y = test_rmse_mean, color = "cv rmse")) +
  geom_point(
    data = slice_min(boostResult_cv, order_by = test_rmse_mean, n = 1),
    aes(x = iter, y = test_rmse_mean),
    color = "firebrick"
  ) +
  labs(
    title = "Evolution of cv-error vs number of trees",
    x     = "number of trees",
    y     = "cv-error (rmse)",
    color = ""
  ) +
  theme_bw() +
  theme(legend.position = "bottom")
```




```r
paste("Optimal number of rounds (nrounds):", slice_min(boostResult_cv, order_by = test_rmse_mea
```

```
[1] "Optimal number of rounds (nrounds): 77"
```

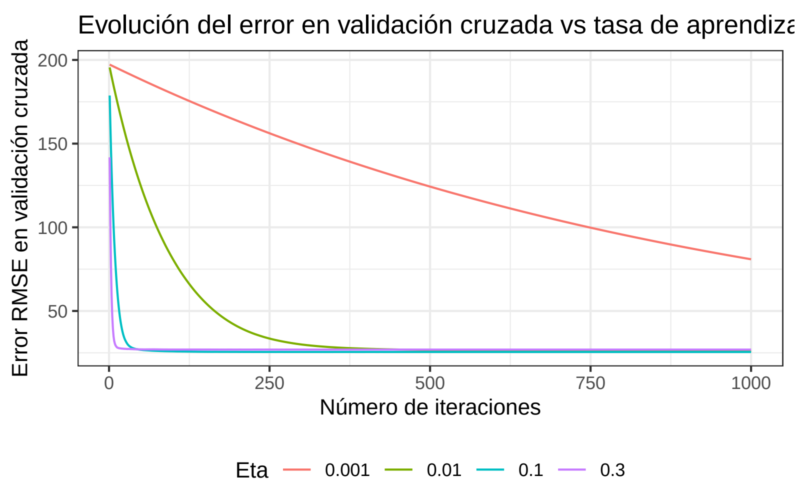
Learning rate

Alongside the number of trees, the learning rate (eta) is the most crucial hyperparameter in Gradient Boosting. It controls how quickly the model learns and thus influences the risk of overfitting.

These two hyperparameters are interdependent: a lower learning rate requires more trees to achieve good results but reduces the risk of overfitting.

```r
# Rango de valores para la tasa de aprendizaje (eta)
eta_range <- c(0.001, 0.01, 0.1, 0.3)
df_results_cv <- data.frame()

for (i in seq_along(eta_range)) {
  set.seed(123)

  # Validación cruzada con el eta actual
  results_cv <- xgb.cv(
    data = ames_train_matrix,  #  Usamos el xgb.DMatrix correcto
    params = list(
      eta = eta_range[i],
      max_depth = 6,
      subsample = 1,
      objective = "reg:squarederror"
    ),
    nrounds = 1000,
    nfold = 5,
    metrics = "rmse",
    verbose = 0
  )

  # Extraer la evaluación de RMSE y registrar resultados
  results_cv <- results_cv$evaluation_log
  results_cv <- results_cv %>%
    select(iter, test_rmse_mean) %>%
    mutate(eta = as.character(eta_range[i]))  # Guardamos el eta usado

  df_results_cv <- df_results_cv %>% bind_rows(results_cv)
}
```

```
ggplot(data = df_results_cv) +
  geom_line(aes(x = iter, y = test_rmse_mean, color = eta)) +
  labs(
    title = "Evolución del error en validación cruzada vs tasa de aprendizaje (eta)",
    x = "Número de iteraciones",
    y = "Error RMSE en validación cruzada",
    color = "Eta"
  ) +
  theme_bw() +
  theme(legend.position = "bottom")
```



Optimized predictor

In order to obtain improved predictors one can perform a a grid search for the best parameter combination can be performed.

```
# Convertir variables categóricas a dummy variables usando model.matrix()
ames_train_num <- model.matrix(Sale_Price ~ . , data = ames_train)[,-1]
ames_test_num <- model.matrix(Sale_Price ~ . , data = ames_test)[,-1]

# Extraer etiquetas de Sale_Price
train_labels <- ames_train$Sale_Price
test_labels <- ames_test$Sale_Price
```

```r
# Convertir a xgb.DMatrix
ames_train_matrix <- xgb.DMatrix(
  data = ames_train_num,
  label = train_labels
)

ames_test_matrix <- xgb.DMatrix(
  data = ames_test_num,
  label = test_labels
)

# Range of parameter values to test
eta_values <- c(0.01, 0.05, 0.1, 0.3)
nrounds_values <- c(500, 1000, 2000)

best_rmse <- Inf
best_params <- list()
```

```r
cv_results_df <- data.frame()

set.seed(123)

for (eta in eta_values) {
  for (nrounds in nrounds_values) {

    cv_results <- xgb.cv(
      data = ames_train_matrix,
      params = list(
        eta = eta,
        max_depth = 6,
        subsample = 0.8,
        colsample_bytree = 0.8,
        objective = "reg:squarederror"
      ),
      nrounds = nrounds,
      nfold = 5,
      metrics = "rmse",
      verbose = 0,
      early_stopping_rounds = 10
    )
```

```r
    if (is.null(cv_results)) next

    results_row <- data.frame(
      eta = eta,
      nrounds = nrounds,
      min_rmse = min(cv_results$evaluation_log$test_rmse_mean),
      best_nrounds = cv_results$evaluation_log$iter[which.min(cv_results$evaluation_log$test_rm
    )

    cv_results_df <- bind_rows(cv_results_df, results_row)

    if (results_row$min_rmse < best_rmse) {
      best_rmse <- results_row$min_rmse
      best_params <- list(
        eta = results_row$eta,
        nrounds = results_row$best_nrounds
      )
    }
  }
}
```

```r
cat("\n, Best hyperparameters values found:\n")
```

```
, Best hyperparameters values found:
```

```r
cat("Eta:", best_params$eta, "\n")
```

```
Eta: 0.01
```

```r
cat("Nrounds:", best_params$nrounds, "\n")
```

```
Nrounds: 1000
```

```r
cat("RMSE mínimo:", round(best_rmse, 4), "\n")
```

```
RMSE mínimo: 24.4476
```

References