Lab 2: Ensembles of Trees

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2026-05-20

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

# Modeling packages
#library(caret)       # for general model fitting
library(rpart)       # for fitting decision trees
library(ipred)       # for fitting bagged decision trees
```

Introduction

This lab presents some examples on building ensemble predictors with a variety of methods.

In order to facilitate the comparison between methods and tools the same prediction problem will be solved with distinct methods and distinct parameter settings.

We will work with the `AmesHousing` dataset, a dataset with multiple variables about housing in Ames, IA. Our goal is to predict the sales prices stored in the `Sale_Price` variable.

The dataset

Package `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)

```
data(ames, package = "modeldata")
dim(ames)
```

```
[1] 2930   74
```

Exploratory Data Analysis and preprocessing

The dataset has 74 variables, and has already been prepared by the package `modeldata`maintainers.

In any case it is always recommended to do some Exploratory Analysis.

```
library(skimr)
skim(ames)
```

Table 1: Data summary

Name	ames
Number of rows	2930
Number of columns	74
_____	
Column type frequency:	
factor	40
numeric	34
_____	
Group variables	None

Variable type: factor

skim_variable	n_missing	complete_rate	ordered	n_unique	top_counts
MS_SubClass	0	1	FALSE	16	One: 1079, Two: 575, One: 287, One: 192

skim_variable	n_missing	complete_rate	ordered	n_unique	top_counts
MS_Zoning	0	1	FALSE	7	Res: 2273, Res: 462, Flo: 139, Res: 27
Street	0	1	FALSE	2	Pav: 2918, Grv: 12
Alley	0	1	FALSE	3	No_: 2732, Gra: 120, Pav: 78
Lot_Shape	0	1	FALSE	4	Reg: 1859, Sli: 979, Mod: 76, Irr: 16
Land_Contour	0	1	FALSE	4	Lvl: 2633, HLS: 120, Bnk: 117, Low: 60
Utilities	0	1	FALSE	3	All: 2927, NoS: 2, NoS: 1
Lot_Config	0	1	FALSE	5	Ins: 2140, Cor: 511, Cul: 180, FR2: 85
Land_Slope	0	1	FALSE	3	Gtl: 2789, Mod: 125, Sev: 16
Neighborhood	0	1	FALSE	28	Nor: 443, Col: 267, Old: 239, Edw: 194
Condition_1	0	1	FALSE	9	Nor: 2522, Fee: 164, Art: 92, RRA: 50
Condition_2	0	1	FALSE	8	Nor: 2900, Fee: 13, Art: 5, Pos: 4
Bldg_Type	0	1	FALSE	5	One: 2425, Twn: 233, Dup: 109, Twn: 101
House_Style	0	1	FALSE	8	One: 1481, Two: 873, One: 314, SLv: 128
Overall_Cond	0	1	FALSE	9	Ave: 1654, Abo: 533, Goo: 390, Ver: 144
Roof_Style	0	1	FALSE	6	Gab: 2321, Hip: 551, Gam: 22, Fla: 20
Roof_Matl	0	1	FALSE	8	Com: 2887, Tar: 23, WdS: 9, WdS: 7
Exterior_1st	0	1	FALSE	16	Vin: 1026, Met: 450, HdB: 442, Wd : 420
Exterior_2nd	0	1	FALSE	17	Vin: 1015, Met: 447, HdB: 406, Wd : 397
Mas_Vnr_Type	0	1	FALSE	5	Non: 1775, Brk: 880, Sto: 249, Brk: 25

skim_variable	n_missing	complete_rate	ordered	n_unique	top_counts
Exter_Cond	0	1	FALSE	5	Typ: 2549, Goo: 299, Fai: 67, Exc: 12
Foundation	0	1	FALSE	6	PCo: 1310, CBl: 1244, Brk: 311, Sla: 49
Bsmt_Cond	0	1	FALSE	6	Typ: 2616, Goo: 122, Fai: 104, No_: 80
Bsmt_Exposure	0	1	FALSE	5	No: 1906, Av: 418, Gd: 284, Mn: 239
BsmtFin_Type_1	0	1	FALSE	7	GLQ: 859, Unf: 851, ALQ: 429, Rec: 288
BsmtFin_Type_2	0	1	FALSE	7	Unf: 2499, Rec: 106, LwQ: 89, No_: 81
Heating	0	1	FALSE	6	Gas: 2885, Gas: 27, Gra: 9, Wal: 6
Heating_QC	0	1	FALSE	5	Exc: 1495, Typ: 864, Goo: 476, Fai: 92
Central_Air	0	1	FALSE	2	Y: 2734, N: 196
Electrical	0	1	FALSE	6	SBr: 2682, Fus: 188, Fus: 50, Fus: 8
Functional	0	1	FALSE	8	Typ: 2728, Min: 70, Min: 65, Mod: 35
Garage_Type	0	1	FALSE	7	Att: 1731, Det: 782, Bui: 186, No_: 157
Garage_Finish	0	1	FALSE	4	Unf: 1231, RFn: 812, Fin: 728, No_: 159
Garage_Cond	0	1	FALSE	6	Typ: 2665, No_: 159, Fai: 74, Goo: 15
Paved_Drive	0	1	FALSE	3	Pav: 2652, Dir: 216, Par: 62
Pool_QC	0	1	FALSE	5	No_: 2917, Exc: 4, Goo: 4, Typ: 3
Fence	0	1	FALSE	5	No_: 2358, Min: 330, Goo: 118, Goo: 112

skim_variable	n_missing	complete_rate	ordered	n_unique	top_counts
Misc_Feature	0	1	FALSE	6	Non: 2824, She: 95, Gar: 5, Oth: 4
Sale_Type	0	1	FALSE	10	WD : 2536, New: 239, COD: 87, Con: 26
Sale_Condition	0	1	FALSE	6	Nor: 2413, Par: 245, Abn: 190, Fam: 46

Variable type: numeric

skim_variable	n_missing	complete_rate	mean	sd	p0	p25	p50	p75	p100	hist
Lot_Frontage	0	1	57.65	33.50	0.00	43.00	63.00	78.00	313.00	
Lot_Area	0	1	10147.92	7880.02	1300.00	7440.25	9436.50	11555.25	215245.00	
Year_Built	0	1	1971.36	30.25	1872.00	1954.00	1973.00	2001.00	2010.00	
Year_Remod_Add	0	1	1984.27	20.86	1950.00	1965.00	1993.00	2004.00	2010.00	
Mas_Vnr_Area	1	1	101.10	178.63	0.00	0.00	0.00	162.75	1600.00	
BsmtFin_SF_1	1	1	4.18	2.23	0.00	3.00	3.00	7.00	7.00	
BsmtFin_SF_2	1	1	49.71	169.14	0.00	0.00	0.00	0.00	1526.00	
Bsmt_Unf_SF	1	1	559.07	439.54	0.00	219.00	465.50	801.75	2336.00	
Total_Bsmt_SF	1	1	1051.24	440.97	0.00	793.00	990.00	1301.50	6110.00	
First_Flr_SF	0	1	1159.56	391.89	334.00	876.25	1084.00	1384.00	5095.00	
Second_Flr_SF	0	1	335.46	428.40	0.00	0.00	0.00	703.75	2065.00	
Gr_Liv_Area	0	1	1499.69	505.51	334.00	1126.00	1442.00	1742.75	5642.00	
Bsmt_Full_Bath	1	1	0.43	0.52	0.00	0.00	0.00	1.00	3.00	
Bsmt_Half_Bath	1	1	0.06	0.25	0.00	0.00	0.00	0.00	2.00	
Full_Bath	0	1	1.57	0.55	0.00	1.00	2.00	2.00	4.00	
Half_Bath	0	1	0.38	0.50	0.00	0.00	0.00	1.00	2.00	
Bedroom_AbvGr	0	1	2.85	0.83	0.00	2.00	3.00	3.00	8.00	
Kitchen_AbvGr	0	1	1.04	0.21	0.00	1.00	1.00	1.00	3.00	
TotRms_AbvGrd	0	1	6.44	1.57	2.00	5.00	6.00	7.00	15.00	
Fireplaces	0	1	0.60	0.65	0.00	0.00	1.00	1.00	4.00	
Garage_Cars	1	1	1.77	0.76	0.00	1.00	2.00	2.00	5.00	
Garage_Area	1	1	472.66	215.19	0.00	320.00	480.00	576.00	1488.00	
Wood_Deck_SF	0	1	93.75	126.36	0.00	0.00	0.00	168.00	1424.00	
Open_Porch_SF	0	1	47.53	67.48	0.00	0.00	27.00	70.00	742.00	
Enclosed_Porch	0	1	23.01	64.14	0.00	0.00	0.00	0.00	1012.00	
Three_season_porch	0	1	2.59	25.14	0.00	0.00	0.00	0.00	508.00	
Screen_Porch	0	1	16.00	56.09	0.00	0.00	0.00	0.00	576.00	

skim_variable	n_missing	complete_rate	mean	sd	p0	p25	p50	p75	p100	hist
Pool_Area	0	1	2.24	35.60	0.00	0.00	0.00	0.00	800.00	
Misc_Val	0	1	50.64	566.34	0.00	0.00	0.00	0.00	17000.00	
Mo_Sold	0	1	6.22	2.71	1.00	4.00	6.00	8.00	12.00	
Year_Sold	0	1	2007.79	1.32	2006.00	2007.00	2008.00	2009.00	2010.00	
Sale_Price	0	1	180796.06	79886.69	12789.00	129500.00	160000.00	213500.00	755000.00	
Longitude	0	1	-93.64	0.03	-93.69	-93.66	-93.64	-93.62	-93.58	
Latitude	0	1	42.03	0.02	41.99	42.02	42.03	42.05	42.06	

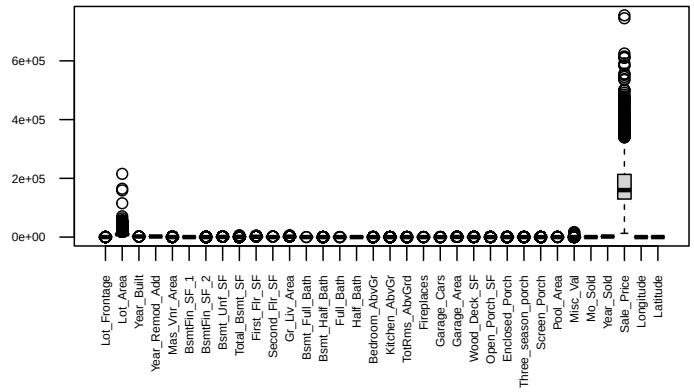
The exploration shows that the data set is well formed with factor data types for categorical variables and no missings.

It can also be seen that the response variable, `Sales_Price` varies on a high range, as confirmed below.

```
summary(ames$Sale_Price)
```

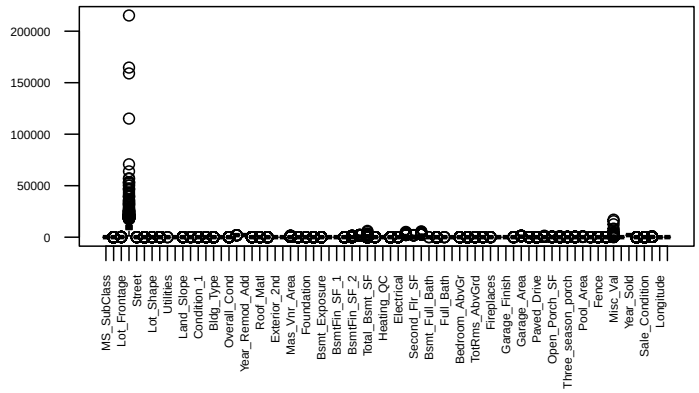
```
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
  12789  129500  160000  180796  213500  755000
```

```
boxplot(ames[,sapply(ames, is.numeric)], las=2, cex.axis=0.5)
```



Although not strictly necessary, given that the variable that has the widest range of variation is the variable to predict we can consider transforming it. In this case the simplest transform seems to express the price in thousands instead of dollars. The distribution of the variable is assymetrical so we may also consider taking logarithm, but given that it would complicate the interpretation of the results, and that something like normality is not required by the methods we use, only division by 1000 is performed.

```
require(dplyr)
ames <- ames %>% mutate(Sale_Price = Sale_Price/1000)
boxplot(ames, las=2, cex.axis=0.5)
```



Spliting the data into test/train

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

```
if(!require(rsample))
  install.packages("rsample", dep=TRUE)
# 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)

dim(ames_train)
```

```
[1] 2049   74
```

```
dim(ames_test)
```

```
[1] 881  74
```

A simple regression tree

As a first attempt to predict `Sales_Price` we build a unique regression tree, which as has been discussed is a weak learner. The `tree` package will be used to fit and optimize the tree.

We build a tree using non-restrictive parameters. This will allow space for pruning it better.

We use the `tree.control` function to set the values for the `control` parameter in the `tree` function.

Let's start with a relatively small tree obtained with mildly restrictive control parameters.

```
library(tree)

# Control pars as defined by tree package
ctl_tree <- tree::tree.control(
  nobs = nrow(ames_train),
  mincut = 5,
  minsize = 10,
  mindev = 0.01
)

ames_rt1 <-  tree::tree(
```

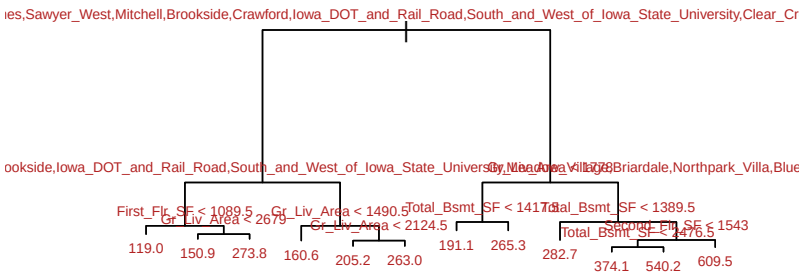
```
                    formula = Sale_Price ~ .,
                    data    = ames_train,
                    split   = "deviance",
                    control = ctl_tree)
summary(ames_rt1)
```

```
Regression tree:
tree::tree(formula = Sale_Price ~ ., data = ames_train, control = ctl_tree,
    split = "deviance")
Variables actually used in tree construction:
[1] "Neighborhood"  "First_Flr_SF"  "Gr_Liv_Area"   "Total_Bsmt_SF"
[5] "Second_Flr_SF"
Number of terminal nodes:  12
Residual mean deviance:  1428 = 2909000 / 2037
Distribution of residuals:
     Min.   1st Qu.    Median      Mean   3rd Qu.      Max.
-227.1000  -21.2400   -0.2372    0.0000   19.0800  212.0000
```

This gives a small tree with only 12 terminal nodes.

We can visualize the tree

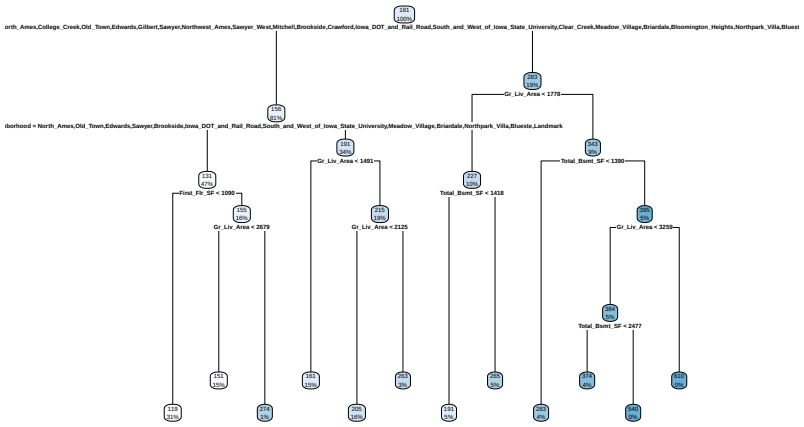
```
plot(x = ames_rt1, type = "proportional")
text(x = ames_rt1, splits = TRUE, pretty = 0, cex = 0.6, col = "firebrick")
```



If instead of using the `tree`package we use `rpart` we can get a better plot. In that case we use the `rpart.control` function to set the values for the `control` parameter in the `rpart` function.

```
# Control pars as defined for package rpart
# Roughly but noty exactly equivalent to ctl_tree
ctl_rpart <- rpart::rpart.control(
  minsplit = 10,
  minbucket = 5,
  cp = 0.01,
  xval = 10
)

ames_rt1bis <- rpart(
  formula = Sale_Price ~ .,
  data    = ames_train,
  method  = "anova",
  control = ctl_rpart
)
```

```
library(rpart.plot)
rpart.plot(ames_rt1bis)
```



Optimizing the tree

In order to optimize the tree we can compute the best cost complexity value

```
set.seed(123)
cv_ames_rt1 <- tree::cv.tree(ames_rt1, K = 5)

optSize <- rev(cv_ames_rt1$size)[which.min(rev(cv_ames_rt1$dev))]
paste("Optimal size obtained is:", optSize)
```

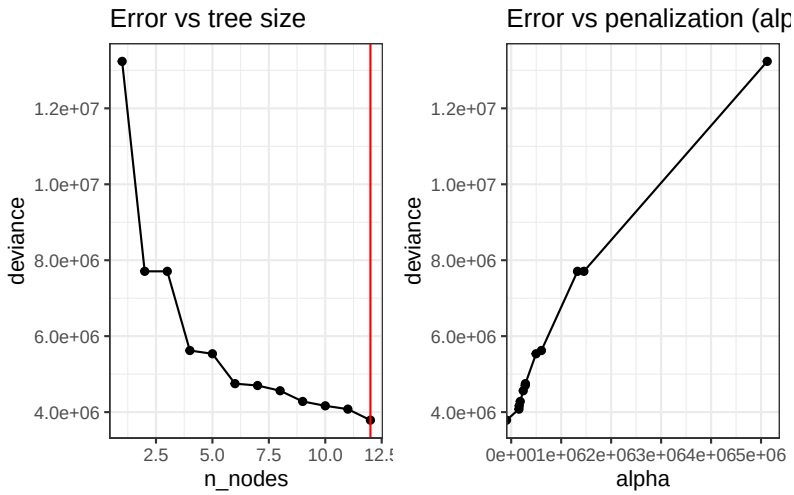
```
[1] "Optimal size obtained is: 12"
```

The optimal tree size coincides with the size of the original tree, *suggesting that pruning would not improve prediction performance.*

This is confirmed by plotting tree size vs deviance which shows that the tree with the smallest error is the biggest one that can be obtained.

```
library(ggplot2)
library(ggpubr)

resultados_cv <- data.frame(
                   n_nodes  = cv_ames_rt1$size,
                   deviance = cv_ames_rt1$dev,
                   alpha    = cv_ames_rt1$k
                 )

p1 <- ggplot(data = resultados_cv, aes(x = n_nodes, y = deviance)) +
      geom_line() +
      geom_point() +
      geom_vline(xintercept = optSize, color = "red") +
      labs(title = "Error vs tree size") +
      theme_bw()

p2 <- ggplot(data = resultados_cv, aes(x = alpha, y = deviance)) +
      geom_line() +
      geom_point() +
```

```
      labs(title = "Error vs penalization (alpha)") +
      theme_bw()

ggarrange(p1, p2)
```



We could have tried to obtain a bigger tree with the hope that pruning might find a better tree. This can be done setting the tree parameters to minimal values.

```
ctl_tree22 <-tree.control(nobs=nrow(ames_train), mincut = 1, minsize = 2, mindev = 0)
ames_rt2 <-  tree::tree(
                    formula = Sale_Price ~ .,
                    data    = ames_train,
                    split   = "deviance",
                    control = ctl_tree22)
summary(ames_rt2)
```

```
Regression tree:
tree::tree(formula = Sale_Price ~ ., data = ames_train, control = ctl_tree22,
    split = "deviance")
Variables actually used in tree construction:
 [1] "Neighborhood"   "First_Flr_SF"   "Garage_Cond"    "Gr_Liv_Area"
 [5] "Central_Air"    "Garage_Area"    "Enclosed_Porch" "Lot_Area"
 [9] "Longitude"      "Latitude"       "MS_SubClass"    "Lot_Frontage"
```

```
[13] "Overall_Cond"   "Year_Built"     "MS_Zoning"      "Alley"
[17] "Fireplaces"     "House_Style"    "BsmtFin_Type_1" "Bsmt_Exposure"
[21] "Bsmt_Unf_SF"    "Electrical"     "Year_Remod_Add" "Exterior_1st"
[25] "Open_Porch_SF"  "Exterior_2nd"   "Functional"     "Mo_Sold"
[29] "Total_Bsmt_SF"  "Bsmt_Full_Bath" "Sale_Condition" "Heating_QC"
[33] "Mas_Vnr_Area"   "Garage_Cars"    "Land_Contour"   "Condition_1"
[37] "Mas_Vnr_Type"   "Second_Flr_SF"  "Lot_Config"     "Exter_Cond"
[41] "Fence"          "Lot_Shape"      "Bsmt_Cond"      "Bedroom_AbvGr"
[45] "Wood_Deck_SF"   "Roof_Style"     "Sale_Type"      "BsmtFin_Type_2"
[49] "Bldg_Type"      "Garage_Type"    "Year_Sold"      "Garage_Finish"
[53] "Screen_Porch"   "Half_Bath"      "Foundation"     "BsmtFin_SF_1"
[57] "Full_Bath"      "Land_Slope"     "TotRms_AbvGrd"
Number of terminal nodes:  1222
Residual mean deviance:  2.579 = 2133 / 827
Distribution of residuals:
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
 -2.750  -0.500   0.000   0.000   0.500   2.943
```

This bigger tree has indeed a smaller deviance but pruning provides no benefit:

```
set.seed(123)
cv_ames_rt2 <- tree::cv.tree(ames_rt2, K = 5)

optSize2 <- rev(cv_ames_rt2$size)[which.min(rev(cv_ames_rt2$dev))]
paste("Optimal size obtained is:", optSize2)
```

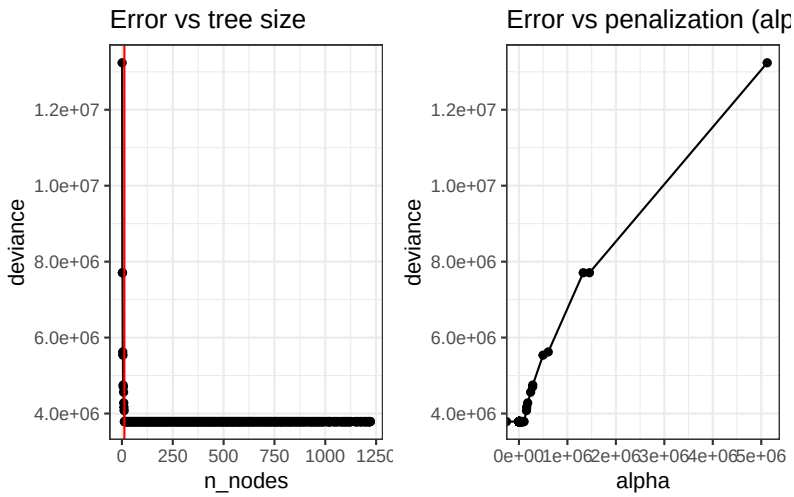
```
[1] "Optimal size obtained is: 12"
```

```
prunedTree2 <- tree::prune.tree(
                   tree = ames_rt2,
                   best = optSize2
                )
summary(prunedTree2)
```

```
Regression tree:
snip.tree(tree = ames_rt2, nodes = c(61L, 31L, 12L, 13L, 60L,
18L, 19L, 14L, 23L, 10L, 22L, 8L))
```

```
Variables actually used in tree construction:
[1] "Neighborhood"  "First_Flr_SF"  "Gr_Liv_Area"   "Total_Bsmt_SF"
[5] "Second_Flr_SF"
Number of terminal nodes:  12
Residual mean deviance:  1428 = 2909000 / 2037
Distribution of residuals:
     Min.   1st Qu.    Median      Mean   3rd Qu.      Max.
-227.1000  -21.2400   -0.2372    0.0000   19.0800  212.0000
```

```r
res_cv2 <- data.frame(
                  n_nodes  = cv_ames_rt2$size,
                  deviance = cv_ames_rt2$dev,
                  alpha    = cv_ames_rt2$k
                 )

p1 <- ggplot(data = res_cv2, aes(x = n_nodes, y = deviance)) +
      geom_line() +
      geom_point() +
      geom_vline(xintercept = optSize2, color = "red") +
      labs(title = "Error vs tree size") +
      theme_bw()

p2 <- ggplot(data = res_cv2, aes(x = alpha, y = deviance)) +
      geom_line() +
      geom_point() +
      labs(title = "Error vs penalization (alpha)") +
      theme_bw()

ggarrange(p1, p2)
```



The performance of the trees is hardly different between small or big tree in pruned or non-pruned version.

```
ames_rt_pred1 <- predict(ames_rt1, newdata = ames_test)
test_rmse1    <- sqrt(mean((ames_rt_pred1 - ames_test$Sale_Price)^2))
paste("Error test (rmse) for initial tree:", round(test_rmse1,2))
```

```
[1] "Error test (rmse) for initial tree: 39.69"
```

```
ames_rt_pred2 <- predict(ames_rt2, newdata = ames_test)
test_rmse2    <- sqrt(mean((ames_rt_pred2 - ames_test$Sale_Price)^2))
paste("Error test (rmse) for big tree:", round(test_rmse2,2))
```

```
[1] "Error test (rmse) for big tree: 37.59"
```

```
ames_pruned_pred <- predict(prunedTree2, newdata = ames_test)
test_rmse3    <- sqrt(mean((ames_pruned_pred - ames_test$Sale_Price)^2))
paste("Error test (rmse) for pruned tree:", round(test_rmse3,2))
```

```
[1] "Error test (rmse) for pruned tree: 39.69"
```

```
improvement <- (test_rmse3-test_rmse2)/test_rmse2*100
```

The MSE for each model will be saved to facilitate comparison with other models

```
errTable <- data.frame(Model=character(),  RMSE=double())
errTable[1, ] <-  c("Default Regression Tree", round(test_rmse1,2))
errTable[2, ] <-  c("Big Regression Tree", round(test_rmse2,2))
errTable[3, ] <-  c("Optimally pruned Regression Tree", round(test_rmse3,2))
```

```
# kableExtra::kable(errTable) %>% kableExtra::kable_styling()
knitr::kable(errTable)
```

Model	RMSE
Default Regression Tree	39.69
Big Regression Tree	37.59
Optimally pruned Regression Tree	39.69

In summary, this example illustrates that, for some datasets, increasing tree complexity only leads to marginal improvements in prediction accuracy.

Building a saturated tree only provides a slight improvement of less than 5% in RMSE at the cost of having to use 5 times more variables in a tree with more than 1000 nodes.

This is a good point to consider using an ensemble instead of single trees.

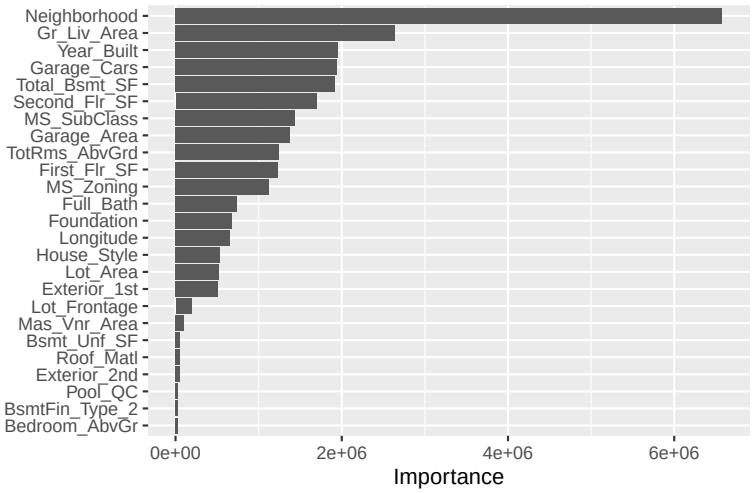
Feature interpretation

To measure feature importance, the reduction in the loss function (e.g., SSE) attributed to each variable at each split is tabulated.

In some instances, a single variable could be used multiple times in a tree; consequently, the total reduction in the loss function across all splits by a variable are summed up and used as the total feature importance.

Not all packages store the informaticon required to compute variable importance. For instance, the `tree`packges does not, but `rpart`or `caret` do save it.

```
vip(ames_rt1bis, num_features = 40, bar = FALSE)
```



Bagging trees

The first attempt to build an ensemble may be to apply `bagging` that is building multiple trees from a set of resamples and averaging the predictions of each tree.

In this example, rather than use a single pruned decision tree, we can use, say, 100 bagged unpruned trees (by not pruning the trees we're keeping bias low and variance high which is when bagging will have the biggest effect).

Bagging can be seen as a particular case of Random Forests *where all predictors are considered at each split.*

Therefore, bagging can be implemented using the `randomForest` package by setting `mtry` equal to the total number of predictors.

```
# make bootstrapping reproducible
set.seed(123)

library(randomForest)
bag.Ames <- randomForest(Sale_Price ~ .,
```

```
                          data = ames_train,
                          mtry = ncol(ames_train)-1,
                          ntree = 100,
                          importance = TRUE)
show(bag.Ames)
```

```
Call:
 randomForest(formula = Sale_Price ~ ., data = ames_train, mtry = ncol(ames_train) -      1, nt
               Type of random forest: regression
                     Number of trees: 100
No. of variables tried at each split: 73

          Mean of squared residuals: 737.1328
                    % Var explained: 88.57
```

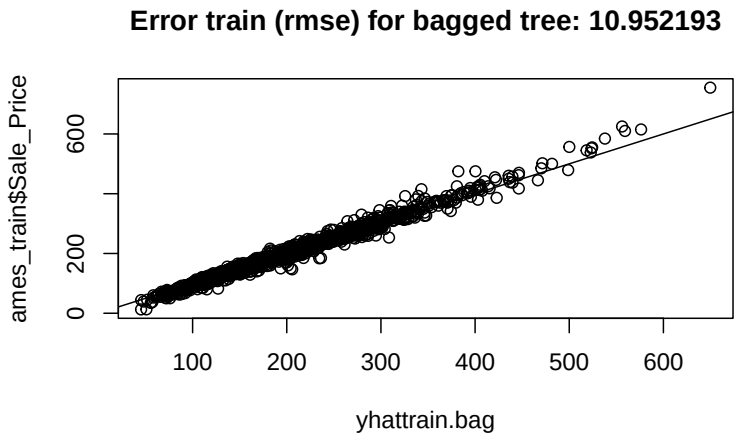
Bagging, as most ensemble procedures, can be time consuming. See Boehmke and Greenwell (2020) for an example on how to easily parallelize code, and save time.

Distinct error rates

The following chunks of code show the fit between data and predictions for the train set, the test set and the out-of bag samples

Error estimated from train samples

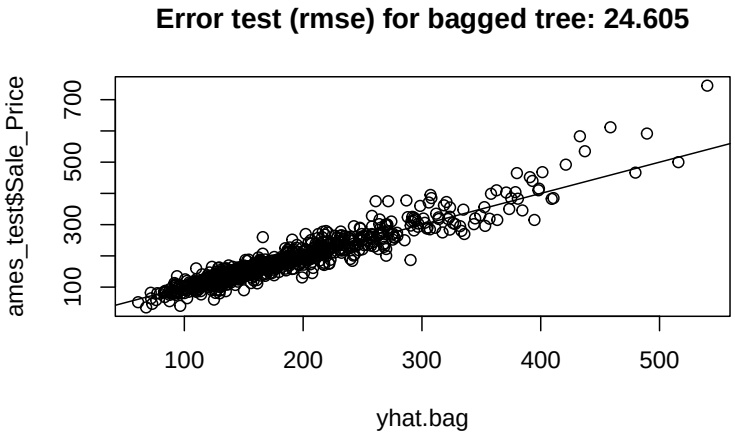
```
yhattrain.bag <- predict(bag.Ames, newdata = ames_train)
# train_mse_bag  <- sqrt(mean(yhattrain.bag - ames_train$Sale_Price)^2)
train_rmse_bag <- sqrt(mean((yhattrain.bag - ames_train$Sale_Price)^2))
showError<- paste("Error train (rmse) for bagged tree:", round(train_rmse_bag,6))
plot(yhattrain.bag, ames_train$Sale_Price, main=showError)
abline(0, 1)
```



As expected, the training error is substantially smaller than the test error because the ensemble adapts very closely to the training data.

Error estimated from test samples

```
yhat.bag <- predict(bag.Ames, newdata = ames_test)
# test_mse_bag  <- sqrt(mean(yhat.bag - ames_test$Sale_Price)^2)
test_rmse_bag  <- sqrt(mean((yhat.bag - ames_test$Sale_Price)^2))
showError<- paste("Error test (rmse) for bagged tree:", round(test_rmse_bag,4))
plot(yhat.bag, ames_test$Sale_Price, main=showError)
abline(0, 1)
```



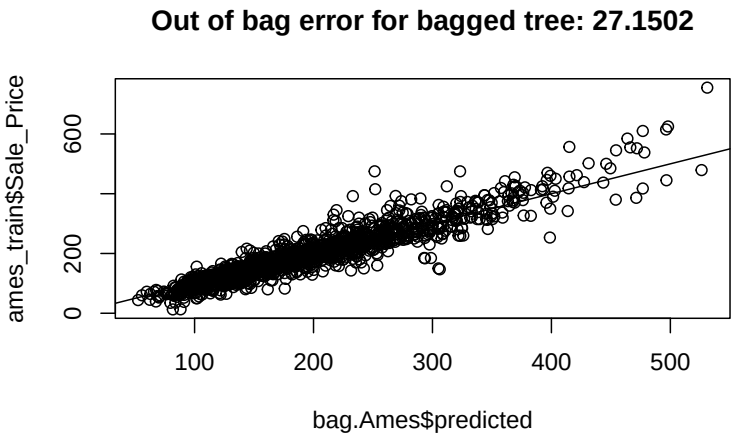
Error estimated from out-of-bag samples

Bagging allows computing an out-of bag error estimate.

For each observation, only the trees where that observation was not included in the bootstrap sample are used to compute its prediction.

Therefore, OOB predictions behave similarly to predictions obtained from an internal validation set, providing an almost unbiased estimate of test error without requiring a separate validation dataset.

```
oob_err<- sqrt(mean((bag.Ames$predicted-ames_train$Sale_Price)^2))
showError <- paste("Out of bag error for bagged tree:", round(oob_err,4))
plot(bag.Ames$predicted, ames_train$Sale_Price, main=showError)
abline(0, 1)
```



Interestingly this may be not only bigger than the error estimated on the train set but also bigger than the error estimated on the test set.

We can collect error rates and compare to each other and also to those obtained from regression trees:

```
errTable <- data.frame(Model=character(),  RMSE=double())
errTable[1, ] <-  c("Default Regression Tree", round(test_rmse1,2))
errTable[2, ] <-  c("Big Regression Tree", round(test_rmse2,2))
errTable[3, ] <-  c("Optimally pruned Regression Tree", round(test_rmse3,2))
errTable[4, ] <-  c("Bagged Tree with Train Data", round(train_rmse_bag,2))
errTable[5, ] <-  c("Bagged Tree with Test Data", round(test_rmse_bag,2))
errTable[6, ] <-  c("Bagged Tree with OOB error rate", round(oob_err,2))
```

Bagging parameter tuning

Bagging tends to improve quickly as the number of resampled trees increases, and then it reaches a plattform.

The figure below has been produced iterated the computation above over `nbagg` values of 1–200 and applied the `bagging()` function.

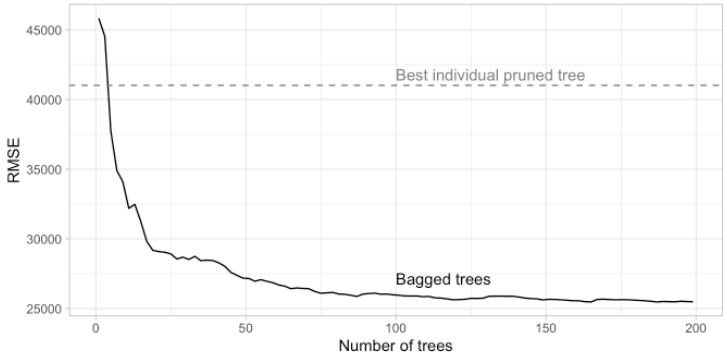


Figure 1: Error curve for bagging 1-200 deep, unpruned decision trees. The benefit of bagging is optimized at 187 trees although the majority of error reduction occurred within the first 100 trees

Variable importance

Due to the bagging process, models that are normally perceived as interpretable are no longer so.

However, we can still make inferences about how features are influencing our model using *feature importance* measures based on the sum of the reduction in the loss function (e.g., SSE) attributed to each variable at each split in a given tree.

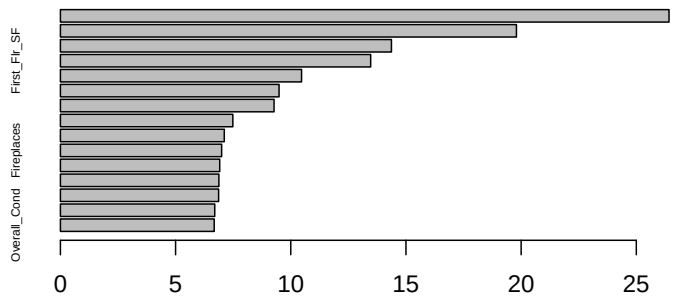
```
require(dplyr)
VIP <- importance(bag.Ames)
VIP <- VIP[order(VIP[,1], decreasing = TRUE),]
head(VIP, n=30)
```

```
                %IncMSE IncNodePurity
Gr_Liv_Area    26.419428    1923769.45
Neighborhood   19.795920    5243520.37
Total_Bsmt_SF  14.370182    1012412.95
First_Flr_SF   13.467640     511525.12
MS_SubClass    10.468429     146349.46
BsmtFin_Type_1  9.491046      57870.21
Year_Remod_Add  9.273779     214595.97
Garage_Area     7.485364     334439.51
```

```
Year_Built      7.112852     266905.91
Fireplaces      6.999228      57043.18
Garage_Cars     6.915052    1777310.87
Bsmt_Unf_SF     6.879415      78882.32
Second_Flr_SF   6.867619     103373.55
Exterior_1st    6.699528      95407.73
Overall_Cond    6.676218      96814.53
Garage_Cond     6.622676      49944.12
Exterior_2nd    5.907220      61992.47
Latitude        5.872897      72448.76
Lot_Area        5.696540     134015.35
Longitude       5.055073      71328.45
Garage_Type     4.686528      37116.56
BsmtFin_SF_1    4.543646      10169.18
Bsmt_Exposure   4.500273      48517.30
Full_Bath       4.416821      84402.03
Garage_Finish   4.405324      24862.60
Sale_Condition  4.173237      25932.41
TotRms_AbvGrd   4.162582      27350.80
Central_Air     4.080131      21049.07
Heating_QC      3.922138      19705.37
Mas_Vnr_Area    3.862446      72973.11
```

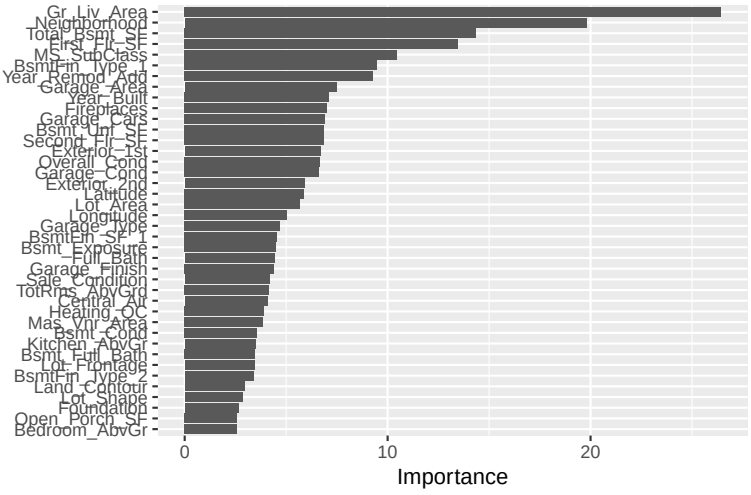
Importance values can be plotted directly:

```
invVIP <-VIP[order(VIP[,1], decreasing = FALSE),1]
tVIP<- tail(invVIP, n=15)
barplot(tVIP, horiz = TRUE, cex.names=0.5)
```



Alternatively one can use the `vip`function from the `vip` package

```
library(vip)
vip(bag.Ames, num_features = 40, bar = FALSE)
```



A random forest to improve bagging

Bagging can be improved if, instead of using all variables to build each tree we rely on subsets of variables, which are chosen

at each split in order to decrease correlation between trees.

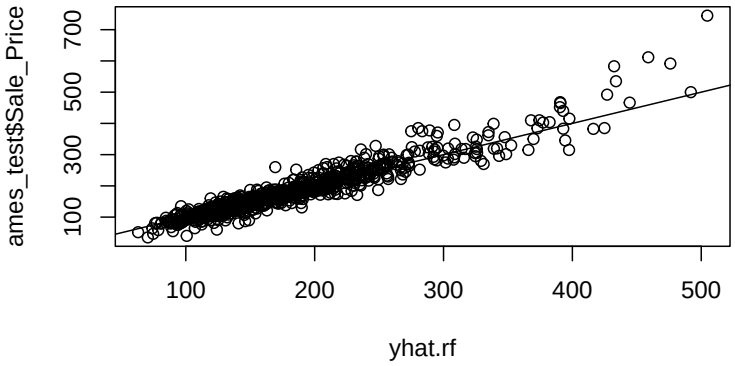
Random Forests are considered to produce good predictors with default values so no parameter is set in a first iteration.

```
# make bootstrapping reproducible
set.seed(123)

require(randomForest)
RF.Ames <- randomForest(Sale_Price ~ .,
                        data = ames_train,
                        importance = TRUE)
```

```
show(RF.Ames)
```

```
Call:
 randomForest(formula = Sale_Price ~ ., data = ames_train, importance = TRUE)
               Type of random forest: regression
                     Number of trees: 500
No. of variables tried at each split: 24

          Mean of squared residuals: 729.7088
                    % Var explained: 88.69
```

```
yhat.rf <- predict(RF.Ames, newdata = ames_test)
plot(yhat.rf, ames_test$Sale_Price)
abline(0, 1)
```




```
test_rmse_rf  <- sqrt(mean((yhat.rf - ames_test$Sale_Price)^2))
paste("Error test (rmse) for Random Forest:", round(test_rmse_rf,2))
```

```
[1] "Error test (rmse) for Random Forest: 24.57"
```

```
errTable[7, ] <-  c("Random Forest (defaults)", round(test_rmse_rf,2))
```

There is some improvement on bagging but it is clearly small.

Notice however that the percentage of explained variance is bigger for RF than for Bag

Parameter optimization for RF

Several parameters can be changed to optimize a random forest predictor, but, usually, the most important one is the *number of variables* to be randomly selected at each split m_{try}, followed by the number of tree, which tends to stabilize after a certain value.

A common strategy to find the optimum combination of parameters is to perform a *grid search* through a combination of parameter values. Obviously it can be time consuming so a small grid is run in the example below to illustrate how to do it.

```
num_trees_range <- c(100, 300)
num_vars_range <- c(18, 24, 37)

RFerrTable <- data.frame(Model=character(),
                         NumTree=integer(), NumVar=integer(),
                         RMSE=double())
errValue <- 1
tuneRF <- TRUE
if (tuneRF){
  system.time(
  for (i in seq_along(num_trees_range)){
    for (j in seq_along(num_vars_range)) {
      numTrees <- num_trees_range[i]
      numVars <- num_vars_range [j] # floor(ncol(ames_train)/3) # default
      RF.Ames.n <- randomForest(Sale_Price ~ .,
                           data = ames_train,
                           mtry = numVars,
                           ntree= numTrees,
                           importance = TRUE)
      yhat.rf <- predict(RF.Ames.n, newdata = ames_test)
      oob.rf <- RF.Ames.n$predicted

      test_rmse_rf  <- sqrt(mean((yhat.rf - ames_test$Sale_Price)^2))

      RFerrTable[errValue, ] <-  c("Random Forest",
                             NumTree = numTrees, NumVar = numVars,
                             RMSE = round(test_rmse_rf,2))
      errValue <- errValue+1
    }
  }
  )
  save(RFerrTable, file="RFerrTable.Rda")
}else{
  load(file="RFerrTable.Rda")
}
```

```
RFerrTable %>% knitr::kable()
```

Model	NumTree	NumVar	RMSE
Random Forest	100	18	24.77
Random Forest	100	24	24.71
Random Forest	100	37	25.02
Random Forest	300	18	25.01
Random Forest	300	24	24.7
Random Forest	300	37	24.51

The minimum RMSE is attained at.

```
bestRF <- which(RFerrTable$RMSE==min(RFerrTable$RMSE))
RFerrTable[bestRF,]
```

```
          Model NumTree NumVar  RMSE
6 Random Forest     300     37 24.51
```

```
minRFErr <- as.numeric(RFerrTable[bestRF,4])
errTable[8, ] <-  c("Random Forest (Optimized)", round(minRFErr,2))
```

Error comparison for all approaches

```
# kableExtra::kable(errTable) %>% kableExtra::kable_styling()
knitr::kable(errTable)
```

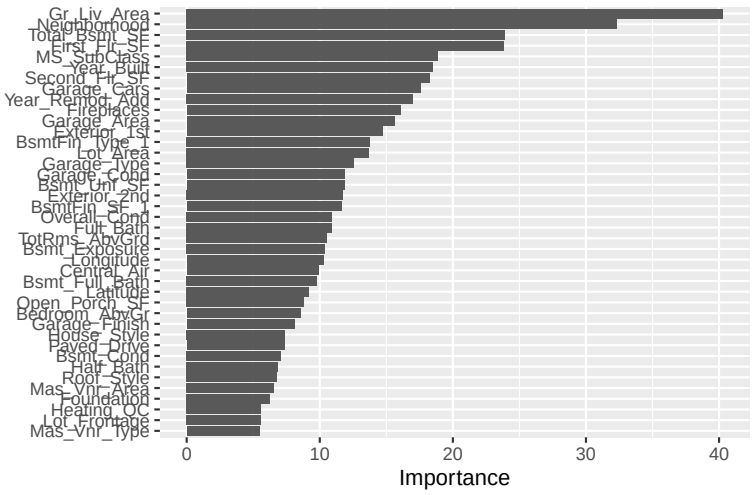
Model	RMSE
Default Regression Tree	39.69
Big Regression Tree	37.59
Optimally pruned Regression Tree	39.69
Bagged Tree with Train Data	10.95
Bagged Tree with Test Data	24.6
Bagged Tree with OOB error rate	27.15
Random Forest (defaults)	24.57
Random Forest (Optimized)	24.51

In summary, it has been shown that the best RMSE was obtained using 37 variables at each split, while increasing the number of trees beyond 100 provided almost no improvement, and even the improvement of the bagging approach is very small. This may be seen as a confirmation from the fact that Random Forests are well known to be good "out-of-the-box predictors", that is that they perform well, even without tuning.

Variable importance

As could be expected, a variable importance plot shows that there is hardly any difference between the variables by bagging or random forests.

```
library(vip)
vip(RF.Ames, num_features = 40, bar = FALSE)
```



Fitting a boosted regression tree with `xgboost`

XGBoost Parameters Overview

The `xgboost()` function in the XGBoost package trains Gradient Boosting models for regression and classification tasks. Key parameters and hyperparameters include:

- **Parameters**:
  - `params`: List of training parameters.
  - `data`: Training data.
  - `nrounds`: Number of boosting rounds.
  - `watchlist`: Validation set for early stopping.
  - `obj`: Custom objective function.
  - `feval`: Custom evaluation function.
  - `verbose`: Verbosity level.
  - `print_every_n`: Print frequency.
  - `early_stopping_rounds`: Rounds for early stopping.
  - `maximize`: Maximize evaluation metric.
  - `save_period`: Model save frequency.
  - `save_name`: Name for saved model.
  - `xgb_model`: Existing XGBoost model.
  - `callbacks`: List of callback functions.

XGBoost Parameters Overview

Numerous parameters govern XGBoost's behavior. A detailed description of all parameters can be found in the `XGBoost` documentation. Key considerations include those controlling tree growth, model learning rate, and early stopping to prevent overfitting:

- **Parameters**:
  - `booster` [default = gbtree]: Type of weak learner, trees ("gbtree", "dart") or linear models ("gblinear").

- `eta` [default=0.3, alias: learning_rate]: Reduces each tree's contribution by multiplying its original influence by this value.
- `gamma` [default=0, alias: min_split_loss]: Minimum cost reduction required for a split to occur.
- `max_depth` [default=6]: Maximum depth trees can reach.
- `subsample` [default=1]: Proportion of observations used for each tree's training. If less than 1, applies Stochastic Gradient Boosting.
- `colsample_bytree`: Number of predictors considered at each split.
- `nrounds`: Number of boosting iterations, i.e., the number of models in the ensemble.
- `early_stopping_rounds`: Number of consecutive iterations without improvement to trigger early stopping. If NULL, early stopping is disabled. Requires a separate validation set (watchlist) for early stopping.
- `watchlist`: Validation set used for early stopping.
- `seed`: Seed for result reproducibility. Note: use `set.seed()` instead.

Test / Training in xGBoost

XGBoost Data Formats

XGBoost models can work with various data formats, including R matrices.

However, it's advisable to use `xgb.DMatrix`, a specialized and optimized data structure within this library.

```
library(xgboost)

xgb_train_mat <- model.matrix(Sale_Price ~ . - 1, data = ames_train)
xgb_test_mat  <- model.matrix(Sale_Price ~ . - 1, data = ames_test)

xgb_train <- xgb.DMatrix(
  data = xgb_train_mat,
```

```
  label = ames_train$Sale_Price
)

xgb_test <- xgb.DMatrix(
  data = xgb_test_mat,
  label = ames_test$Sale_Price
)
```

Fit the model

```
set.seed(123)

ames.boost <- xgb.train(
  data = xgb_train,
  params = list(
    objective = "reg:squarederror",
    max_depth = 2,
    eta = 0.05
  ),
  nrounds = 1000
)
ames.boost
```

```
##### xgb.Booster
call:
  xgb.train(params = list(objective = "reg:squarederror", max_depth = 2,
    eta = 0.05), data = xgb_train, nrounds = 1000)
# of features: 277
# of rounds:  1000
```

Prediction and model assessment

```
ames.boost.trainpred <- predict(
  ames.boost,
  newdata = xgb_train
)
```

```
ames.boost.pred <- predict(
  ames.boost,
  newdata = xgb_test
)

train_rmseboost <- sqrt(mean(
  (ames.boost.trainpred - getinfo(xgb_train, "label"))^2
))

test_rmseboost <- sqrt(mean(
  (ames.boost.pred - getinfo(xgb_test, "label"))^2
))

paste("Error train (rmse) in XGBoost:", round(train_rmseboost,2))
```

```
[1] "Error train (rmse) in XGBoost: 14.78"
```

```
paste("Error test (rmse) in XGBoost:", round(test_rmseboost,2))
```

```
[1] "Error test (rmse) in XGBoost: 23.6"
```

In summary the comparison of all predictors built up to now:

```
errTable[9, ] <-  c("Boosting with XGBoost (non-Optimized)", round(test_rmseboost,2))

# kableExtra::kable(errTable) %>% kableExtra::kable_styling()
knitr::kable(errTable)
```

Model	RMSE
Default Regression Tree	39.69
Big Regression Tree	37.59
Optimally pruned Regression Tree	39.69
Bagged Tree with Train Data	10.95
Bagged Tree with Test Data	24.6
Bagged Tree with OOB error rate	27.15
Random Forest (defaults)	24.57

Model	RMSE
Random Forest (Optimized)	24.51
Boosting with XGBoost (non-Optimized)	23.6

Questions

Questions

1. Compare the predictive performance obtained with:

   - a single regression tree,
   - Bagging,
   - Random Forests,
   - and XGBoost.

   Which method achieves the lowest test RMSE on the Ames Housing dataset?

2. Compare the training RMSE and the test RMSE for:

   - a single tree,
   - Bagging,
   - Random Forests,
   - and XGBoost.

   Which method appears to overfit the most?

3. Compare the Out-Of-Bag (OOB) error estimate obtained with Bagging to the test RMSE.

   - Are both values similar?
   - Why can OOB error estimation be useful in practice?

4. Inspect the selected value of `mtry` (R) or `max_features` (Python) in the Random Forest model.

   - What value was selected?
   - How does it compare with the total number of predictors?

5. Increase the number of trees (`ntree` in R or `n_estimators` in Python) from 100 to 1000 in the Random Forest model.

   - Does predictive performance improve substantially?
   - Does computation time increase noticeably?

6. Identify the 10 most important variables according to the Random Forest model.

   - Are these variables reasonable from a real-estate perspective?
   - Do the same variables appear important in both R and Python?

7. Compare the variable importance rankings obtained from:

   - Bagging,
   - Random Forests,
   - and XGBoost (if available).

   Are the same variables consistently important?

8. Train a Random Forest using only the 10 most important predictors identified previously.

   - How much predictive performance is lost compared with the full model?

9. Modify the Random Forest model so that only numerical predictors are used.

   - Does predictive performance decrease?
   - Which categorical variables seem most informative in the original model?

10. Change the value of `max_features` (`mtry`) manually in the Random Forest model:

    - try a very small value,
    - and a very large value.

    How does this affect:

    - test RMSE,

- and the diversity of trees?

11. In the XGBoost model, modify the value of:

    - `eta`,
    - `max_depth`,
    - or `nrounds`.

    Which parameter appears to have the strongest effect on predictive performance?

12. Increase the number of boosting rounds (`nrounds`) in XGBoost.

    - Does the training RMSE continue decreasing?
    - Does the test RMSE eventually stop improving?

13. Compare the predictions versus observed values plots for:

    - Bagging,
    - Random Forests,
    - and XGBoost.

    Which method appears to produce the most homogeneous prediction errors?

14. Repeat the train/test split using a different random seed.

    - Are the results stable?
    - Which method appears most robust to changes in the split?

15. Compare the execution time of:

    - a single regression tree,
    - Bagging,
    - Random Forests,
    - and XGBoost.

    Is the increase in predictive performance worth the additional computational cost?

16. In the Python notebook, inspect the effect of `OneHotEncoder`.

- How many predictors are generated after preprocessing?
- Why is this transformation necessary in `scikit-learn` but not explicitly required in most R tree implementations?

17. Compare the ensemble implementations in R and Python.

    - Are the results identical?
    - Which implementation is easier to customize or interpret?

References

Boehmke, Bradley, and Brandon Greenwell. 2020. *The r Series Hands-on Machine Learning with r. CRC Press.* https://www.routledge.com/Hands-On-Machine-Learning-with-R/Boehmke-Greenwell/p/book/9781138495685.