

Lab 2: Ensembles of Trees

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```
# 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 an 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 | n_complete | n_ordered | n_unique | top_counts |
|---------------|-----------|------------|-----------|---|------------|
| MS_SubClass0 | 1 | FALSE | 16 | One: 1079, Two: 575, One: 287, One: 192 | |

| skim_variable | missing | complete | ordered | 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 | missing | complete | ordered | 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 | ordered | unique | top_counts |
|-----------------|-----------|----------|---------|---|------------|
| Misc_Feature0 | 1 | FALSE | 6 | Non: 2824, She: 95, Gar: 5, Oth: 4 | |
| Sale_Type0 | 1 | FALSE | 10 | WD : 2536, New: 239, COD: 87, Con: 26 | |
| Sale_Condition0 | 1 | FALSE | 6 | Nor: 2413, Par: 245, Abn: 190, Fam: 46 | |

Variable type: numeric

| skim_variable | n_missing | complete | mean | std | p0 | p25 | p50 | p75 | p100 | hist |
|--------------------|-----------|-------------|---------|---------|--------|---------|---------|---------|------|------|
| Lot_Frontage | 1 | 57.65 | 33.500 | 0.00 | 43.00 | 63.00 | 78.00 | 313.00 | | |
| Lot_Area0 | 1 | 101477880.0 | 1200.70 | 40.25 | 136.50 | 155525 | 245.00 | | | |
| Year_Built | 1 | 1971.36 | 0.25 | 1872.09 | 54.09 | 73.00 | 01.00 | 10.00 | | |
| Year_Remod_Add | 1 | 1984.27 | 0.86 | 1950.09 | 65.09 | 93.00 | 04.00 | 10.00 | | |
| Mas_Vnr_Area | 1 | 101.10 | 178.63 | 0.00 | 0.00 | 0.00 | 162.75 | 1600.00 | | |
| BsmtFin_SF_1 | 1 | 4.18 | 2.23 | 0.00 | 3.00 | 3.00 | 7.00 | 7.00 | | |
| BsmtFin_SF_2 | 1 | 49.71 | 169.14 | 0.00 | 0.00 | 0.00 | 0.00 | 1526.00 | | |
| Bsmt_Unf_SF | 1 | 559.07 | 139.50 | 0.00 | 219.00 | 465.50 | 801.75 | 2336.00 | | |
| Total_Bsmt_SF | 1 | 1051.26 | 10.90 | 0.00 | 793.00 | 990.00 | 1301.50 | 110.00 | | |
| First_Flr_SF | 1 | 1159.59 | 1.83 | 34.08 | 76.25 | 1084.00 | 1384.00 | 995.00 | | |
| Second_Flr_SF | 1 | 335.46 | 128.40 | 0.00 | 0.00 | 0.00 | 703.75 | 2065.00 | | |
| Gr_Liv_Area | 1 | 1499.60 | 5.53 | 34.00 | 126.00 | 442.00 | 742.75 | 42.00 | | |
| Bsmt_Full_Bath | 1 | 0.43 | 0.52 | 0.00 | 0.00 | 0.00 | 1.00 | 3.00 | | |
| Bsmt_Half_Bath | 1 | 0.06 | 0.25 | 0.00 | 0.00 | 0.00 | 0.00 | 2.00 | | |
| Full_Bath0 | 1 | 1.57 | 0.55 | 0.00 | 1.00 | 2.00 | 2.00 | 4.00 | | |
| Half_Bath0 | 1 | 0.38 | 0.50 | 0.00 | 0.00 | 0.00 | 1.00 | 2.00 | | |
| Bedroom_AbvGr | 1 | 2.85 | 0.83 | 0.00 | 2.00 | 3.00 | 3.00 | 8.00 | | |
| Kitchen_AbvGr | 1 | 1.04 | 0.21 | 0.00 | 1.00 | 1.00 | 1.00 | 3.00 | | |
| TotRms_AbvGr | 1 | 6.44 | 1.57 | 2.00 | 5.00 | 6.00 | 7.00 | 15.00 | | |
| Fireplaces0 | 1 | 0.60 | 0.65 | 0.00 | 0.00 | 1.00 | 1.00 | 4.00 | | |
| Garage_Cars | 1 | 1.77 | 0.76 | 0.00 | 1.00 | 2.00 | 2.00 | 5.00 | | |
| Garage_Area | 1 | 472.60 | 15.19 | 0.00 | 320.00 | 480.00 | 576.00 | 1488.00 | | |
| Wood_Deck_SF | 1 | 93.75 | 126.36 | 0.00 | 0.00 | 0.00 | 168.00 | 1424.00 | | |
| Open_Porch_SF | 1 | 47.53 | 67.48 | 0.00 | 0.00 | 27.00 | 70.00 | 742.00 | | |
| Enclosed_Porch | 1 | 23.01 | 64.14 | 0.00 | 0.00 | 0.00 | 0.00 | 1012.00 | | |
| Three_season_porch | 1 | 2.59 | 25.14 | 0.00 | 0.00 | 0.00 | 0.00 | 508.00 | | |
| Screen_Porch | 1 | 16.00 | 56.09 | 0.00 | 0.00 | 0.00 | 0.00 | 576.00 | | |

| skim_variable | missing | complete | mean | std | p0 | p25 | p50 | p75 | p100 | hist |
|---------------|---------|----------|-----------|-----------|---------|---------|---------|---------|----------|------|
| Pool_Area | 0 | 1 | 2.24 | 35.600 | 0.00 | 0.00 | 0.00 | 0.00 | 800.00 | |
| Misc_Val | 0 | 1 | 50.64 | 566.340 | 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 | 2007.7932 | 2006.2007 | 2006.00 | 2007.00 | 2008.00 | 2009.00 | 2010.00 | |
| Sale_Price | 0 | 1 | 180796 | 79861 | 127891 | 129500 | 160000 | 213500 | 755000 | |
| Longitude | 0 | 1 | - | 0.03 | - | - | - | - | - | |
| | | | 93.64 | | 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, **Sale_Price** varies on a high range, as confirmed below.

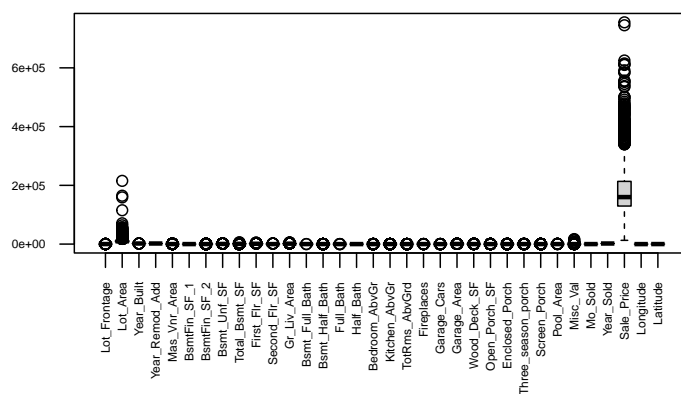
```
summary(ames$Sale_Price)
```

```

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

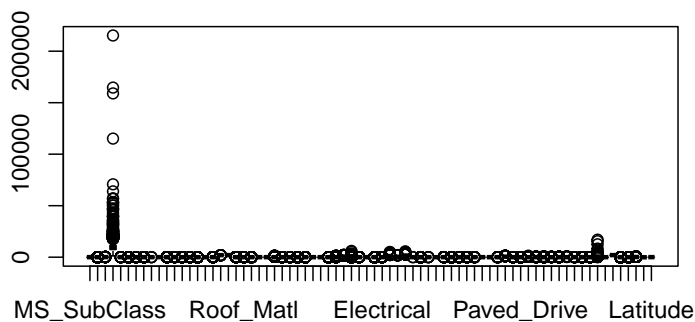
```

```
boxplot(ames[,apply(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 asymmetrical 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)
```



Splitting 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)
```

A simple regression tree

As a first attempt to predict `Sale_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 tree with the default values.

```
library(tree)

ctlPars <- 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 = ctlPars)

summary(ames_rt1)
```

Regression tree:

```
tree::tree(formula = Sale_Price ~ ., data = ames_train, control = ctlPars,
            split = "deviance")
```

Variables actually used in tree construction:

```
[1] "Neighborhood" "First_Flr_SF" "Gr_Liv_Area" "Total_Bsmt_SF"
```



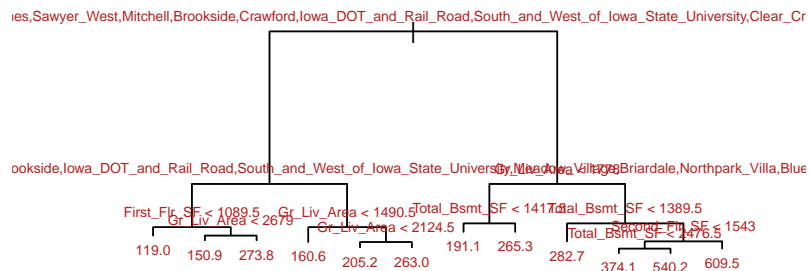
```
[5] "Second_Flr_SF"
Number of terminal nodes: 12
Residual mean deviance: 1428 = 2909000 / 2037
Distribution of residuals:
```

| 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 11 terminal nodes.

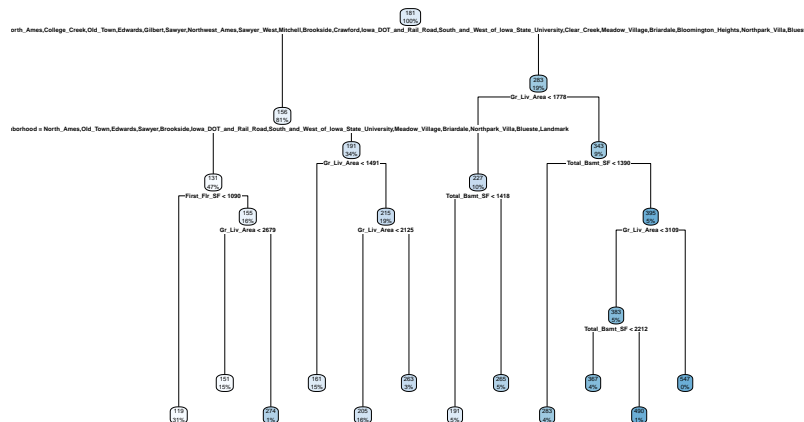
We can visualize the tree

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



If instead of using the `treepackage` we use `rpart` we can get a better plot:

```
ames_rtlbis <- rpart(
  formula = Sale_Price ~ .,
  data     = ames_train,
  method   = "anova",
  control  = ctlPars
)
library(rpart.plot)
rpart.plot(ames_rtlbis)
```



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 best value of α is obtained with the same tree, which suggests that *there will be no advantage in pruning*.

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(
```

```

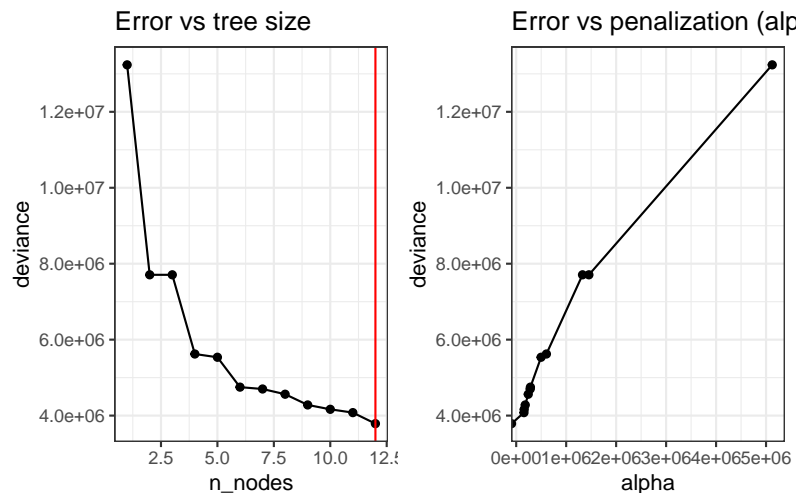
      n_nodes = cv_ames_rt1$size,
      deviance = cv_ames_rt1$dev,
      alpha = cv_ames_rt1$k
    )

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.

```

ctlPars2 <- 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 = ctlPars2)
summary(ames_rt2)

```

Regression tree:

```

tree::tree(formula = Sale_Price ~ ., data = ames_train, control = ctlPars2,
  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 |

```
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()

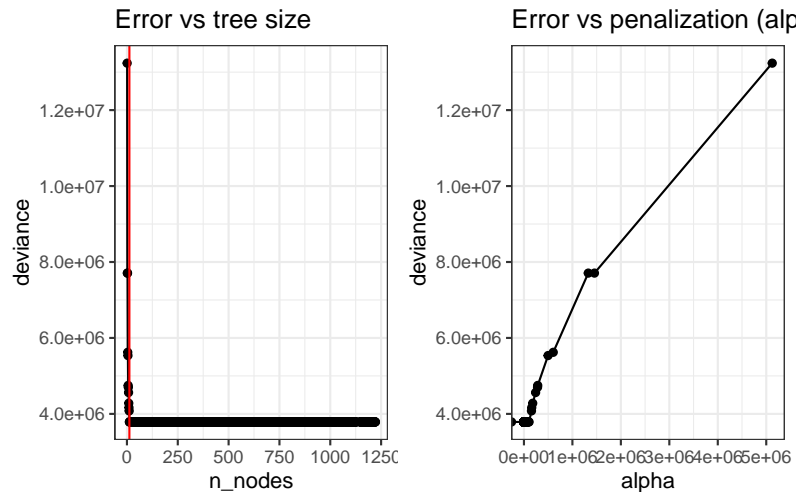
p2 <- ggplot(data = res_cv2, aes(x = alpha, y = deviance)) +
```

```

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, what is illustrated by this example is that, *for some datasets, it is very hard to obtain an optimal tree because there seems to be a minimum complexity which is very hard to decrease.*

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.

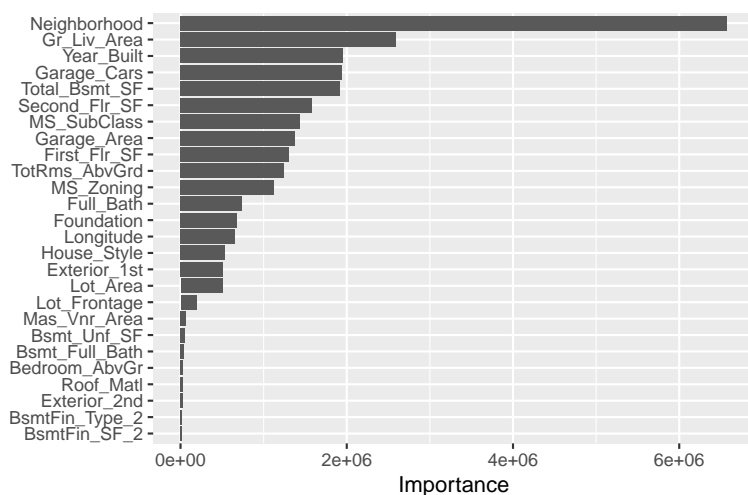
Feature interpretation

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 information required to compute variable importance. For instance, the `treepackages` does not, but `rpart` or `caret` do save it.

```
vip(ames_rtlbis, 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 is equivalent to RandomForest if we use all the trees so the library `randomForest` is used.

```
# 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), n
              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
```

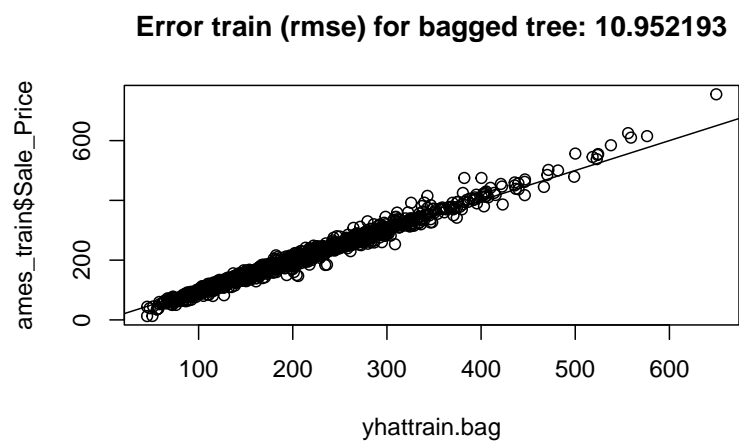
Bagging, as most ensemble procedures, can be time consuming. See [Boehmke and Greenwell \(2020\)](#) for an example on how to easily parallelize code, and save time.

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)
```

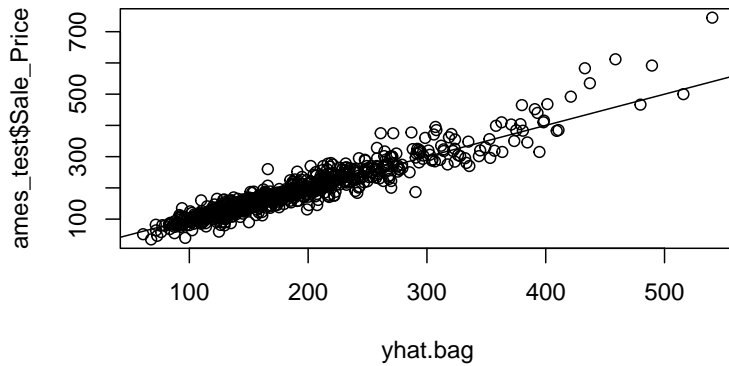


This error is much smaller even than those from trees because of overfitting

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 test (rmse) for bagged tree: 24.605

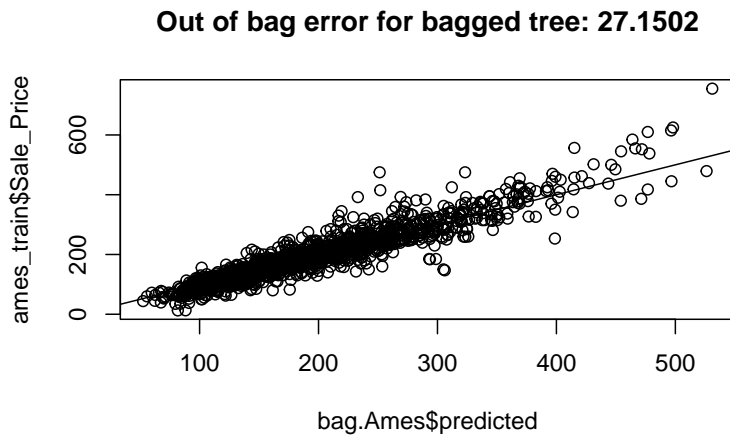


Error estimated from out-of-bag samples

Bagging allows computing an out-of bag error estimate.

Out of bag error rate is reported in the output and can be computed from the `predicted` (*“the predicted values of the input data based on out-of-bag samples”*)

```
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 platform.

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

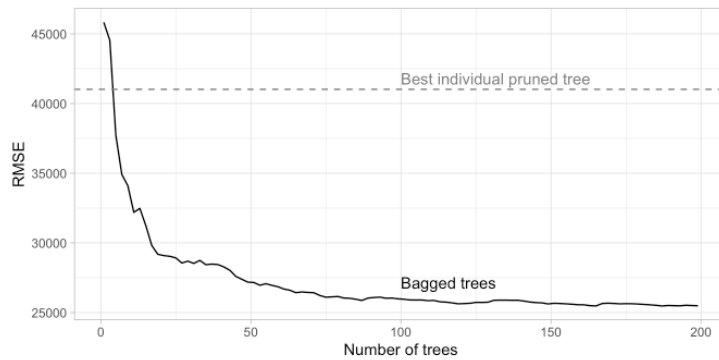


Figure 1: Error curve for bagging 1-200 deep, unpruned decision trees. The benefit of bagging is optimized at 187 trees although the majority of error reduction occurred within the first 100 trees

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)
```


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)

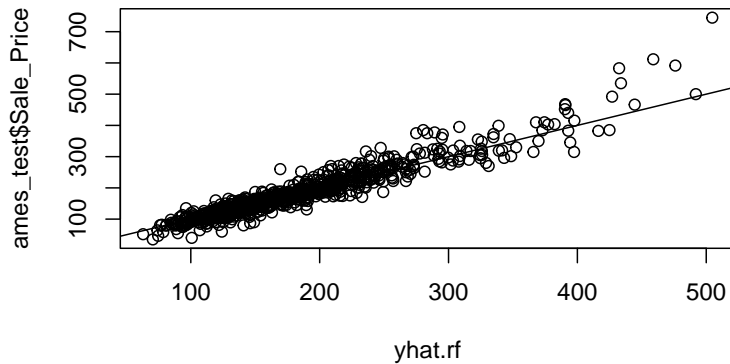
show(RF.Ames)
```

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 <- seq(100, 400, 100)

num_vars_range <- floor(ncol(ames_train)/(seq(2,4,1)))

RFerrTable <- data.frame(Model=character(),
                          NumTree=integer(), NumVar=integer(),
                          RMSE=double())

errValue <- 1
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
  }
}
)

```

```

user  system elapsed
235.81    3.10   251.98

```

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

| Model | NumTree | NumVar | RMSE |
|---------------|---------|--------|-------|
| Random Forest | 100 | 37 | 24.51 |
| Random Forest | 100 | 24 | 24.85 |
| Random Forest | 100 | 18 | 24.79 |
| Random Forest | 200 | 37 | 24.66 |
| Random Forest | 200 | 24 | 24.86 |
| Random Forest | 200 | 18 | 24.74 |
| Random Forest | 300 | 37 | 24.51 |
| Random Forest | 300 | 24 | 24.53 |
| Random Forest | 300 | 18 | 25.12 |
| Random Forest | 400 | 37 | 24.58 |
| Random Forest | 400 | 24 | 24.62 |
| Random Forest | 400 | 18 | 24.84 |

The minimum RMSE is attained at.

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

| | Model | NumTree | NumVar | RMSE |
|---|---------------|---------|--------|-------|
| 1 | Random Forest | 100 | 37 | 24.51 |
| 7 | 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 |

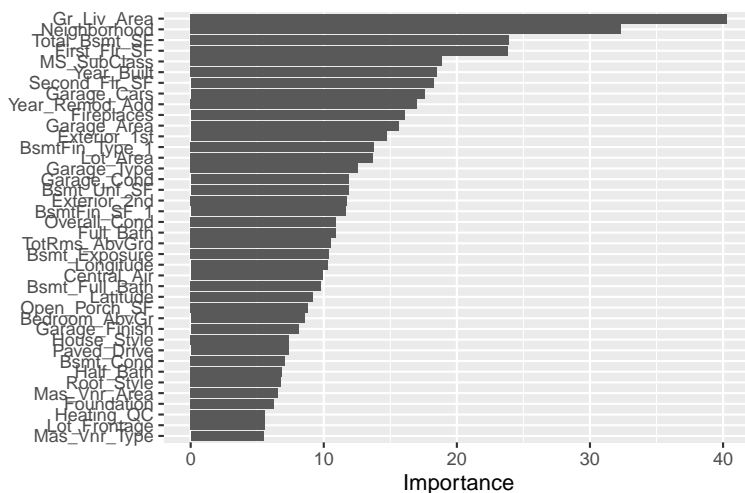
| Model | RMSE |
|---------------------------------|-------|
| Bagged Tree with Train Data | 10.95 |
| Bagged Tree with Test Data | 24.6 |
| Bagged Tree with OOB error rate | 27.15 |
| Random Forest (defaults) | 24.57 |
| Random Forest (Optimized) | 24.51 |

In summary, it has been shown that a Random Forest with 400 trees and 37 variables provides the smallest error rate, though the improvement on the default values and even 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)
```



Random Forests with Python

The following link points to a good brief tutorial on how to train and evaluate Random Forests using Python

[DataCamp: Random Forest Classification with Scikit-Learn](#)

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>.