Random Forests

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Random Forests

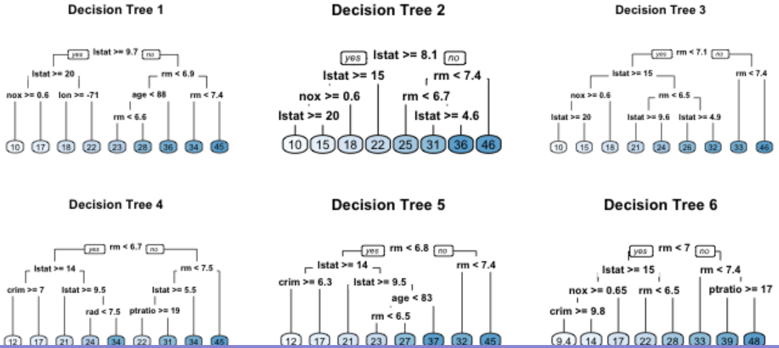
- Thus, **bagging** can turn a single tree model with high variance and poor predictive power into a fairly accurate prediction function.
- But bagging suffers from **tree correlation**, which reduces the overall performance of the model.
- **Random forests** are a modification of bagging that builds a large collection of de-correlated trees
- It is a very popular **out-of-the-box**) learning algorithm that enjoys good predictive performance.

Extending the bagging technique

- Bagging introduces a random component in to the tree building process
- The trees in bagging are not completely independent of each other since all the original predictors are considered at every split of every tree.
- Trees from different bootstrap samples have similar structure to each other (especially at the top of the tree) due to underlying relationships.

Similar trees - tree correlation

- If we create six decision trees with different bootstrapped samples of the Boston housing data, the top of the trees all have a very similar structure.
- Although there are 15 predictor variables to split on, all six trees have both `lstat` and `rm` variables driving the first few splits.



Tree correlation

- Tree correlation prevents bagging from optimally reducing variance of the predictive values.
- To reduce variance further, we need to minimize the amount of correlation between the trees.
- This can be achieved by injecting more randomness into the tree-growing process.

Random forests achieve this in two ways:

1) Bootstrap:
   - Similar to bagging, each tree is grown to a bootstrap resampled data set, which makes them different and decorrelates them.
2) Split-variable randomization:
   - For every split, the search for the split variable is limited to a random subset of m of the p variables.
   - For regression trees, typical default values are $m = p/3$ (tuning parameter).
   - When $m = p$, the randomization is limited (only step 1) and is the same as bagging.

Basic algorithm

The basic algorithm for a regression random forest can be generalized:

```
1.  Given training data set
2.  Select number of trees to build (ntrees)
3.  for i = 1 to ntrees do
4.  |  Generate a bootstrap sample of the original data
5.  |  Grow a regression tree to the bootstrapped data
6.  |  for each split do
7.  |  | Select m variables at random from all p variables
8.  |  | Pick the best variable/split-point among the m
9.  |  | Split the node into two child nodes
10. |  end
11. | Use tree model stopping criteria to determine: tree comple
12. end
```

The algorithm randomly selects a bootstrap sample to train and predictors to use at each split.

Characteristics

- Since bootstrap samples and features are selected randomly at each split, we create a more diverse set of trees, which tends to lessen tree correlation beyond bagged trees and often dramatically increase predictive power.

out-of-bag error

- Similar to bagging, a natural benefit of the bootstrap resampling process is that random forests have an **out-of-bag** (OOB) sample that provides an efficient and reasonable approximation of the test error.
- This provides a built-in validation set without any extra work, and you do not need to sacrifice any of your training data to use for validation.
- We are more efficient identifying the number of trees required to stablize the error rate

Preparation - random forests

- The following slides are based on UC Business Analytics R Programming Guide on **random forests**

```
library(rsample)      # data splitting
library(randomForest) # basic implementation
library(ranger)       # a faster implementation of randomForest
# an aggregator package for performing many
# machine learning models
library(caret)
```

The Ames housing data

```r
set.seed(123)
ames_data <- AmesHousing::ames_raw
```

```r
set.seed(123)
ames_split <- rsample::initial_split(ames_data,prop=.7)
ames_train <- rsample::training(ames_split)
ames_test  <- rsample::testing(ames_split)
```

Basic implementation

- There are over 20 random forest packages in R.
- To demonstrate the basic implementation we illustrate the use of the `randomForest` package, the oldest and most well known implementation of the random forest algorithm in R.
- As your data set grows in size `randomForest` does not scale well (although you can parallelize with `foreach`).
- To explore and compare a variety of tuning parameters we can also find more effective packages.
- The package `ranger` will be presented in the tuning section.

randomForest::randomForest

- `randomForest` can use the formula or separate x, y matrix notation for specifying the model.
- Below we apply the default `randomForest` model using the formal specification.
- The default random forest performs 500 trees and $\frac{\text{features}}{3} = 26$ randomly selected predictor variables at each split.

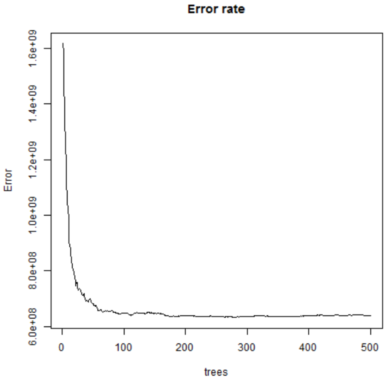
```
set.seed(123)
# default RF model
(m1 <- randomForest(formula = Sale_Price ~ .,data=ames_train))
```

```
##
## Call:
##  randomForest(formula = Sale_Price ~ ., data = ames_train)
##                Type of random forest: regression
##                      Number of trees: 500
## No. of variables tried at each split: 26
##
```

Plotting the model

- The error rate stabalizes with around 100 trees but continues to decrease slowly until around 300 trees.

```
plot(m1,main="Error rate")
```



Random forests - out-of-the-box algorithm

- Random forests perform remarkably well with very little tuning.
- We get an RMSE of less than 30K Dollar without any tuning
- This is more than 6K Dollar RMSE-reduction compared to a fully-tuned bagging model
- and 4K dollar reduction to to a fully-tuned elastic net model.
- We can still seek improvement by tuning our random forest model.

Tuning Random forests

- Random forests are fairly easy to tune since there are only a handful of tuning parameters.
- The primary concern at the beginning is tuning the number of candidate variables to select from at each split.
- A few additional hyperparameters are important.

Tuning parameters (I)

- The argument names may differ across packages, but these hyperparameters should be present:

number of trees

- `ntree` - We want enough trees to stabalize the error but using too many trees is inefficient, esp. for large data sets.

number of variables

- `mtry` - number of variables as candidates at each split. When `mtry=p`the model equates to bagging.
- When `mtry=1` the split variable is completely random, all variables get a chance but can lead to biased results. Suggestion: start with 5 values evenly spaced across the range from 2 to p.

Tuning parameters (II)

Number of samples

- `sampsize` - Default value is 63.25% since this is the expected value of unique observations in the bootstrap sample.
- Lower sample sizes can reduce the training time but may introduce more bias. Increasing sample size can increase performance but at risk of overfitting - it introduces more variance.
- When tuning this parameter we stay near the 60-80% range.

Tuning parameters (III)

minimum number of samples within the terminal nodes:

- `nodesize` - Controls the complexity of the trees.
- Smaller node size allow for deeper, more complex trees
- This is another bias-variance tradeoff where deeper trees introduce more variance (risk of overfitting)
- Shallower trees introduce more bias (risk of not fully capturing unique patters and relatonships in the data).

maximum number of terminal nodes

- `maxnodes`: A way to control the complexity of the trees.
- More nodes equates to deeper, more complex trees.
- Less nodes result in shallower trees.

Initial tuning with randomForest

- If we just tune the `mtry` parameter we can use `randomForest::tuneRF` for a quick and easy tuning assessment.
- We start with 5 candidate variables (`mtryStart=5`) and increase by a factor of 2 until the OOB error stops improving by 1 per cent.
- `tuneRF` requires a separate x y specification.
- The optimal `mtry` value in this sequence is very close to the default mtry value of $\frac{\text{features}}{3} = 26$.

```
features <- setdiff(names(ames_train), "Sale_Price")
```

```
set.seed(123)
m2<-tuneRF(x= ames_train[,features],
  y= ames_train$Sale_Price,ntreeTry   = 500,
  mtryStart  = 5,stepFactor = 2,
  improve    = 0.01,trace=FALSE)
```

Full grid search with `ranger`

- To perform a larger grid search across several hyperparameters we'll need to create a grid, loop through each hyperparameter combination and evaluate the model.
- Unfortunately, this is where `randomForest` becomes quite inefficient since it does not scale well.
- Instead, we can use `ranger` which is a C++ implementation of Breiman's random forest algorithm and is over 6 times faster than `randomForest`.

Assessing the speed

randomForest speed

```
system.time(
  ames_randomForest <- randomForest(
    formula = Sale_Price ~ .,
    data    = ames_train,
    ntree   = 500,
    mtry    = floor(length(features) / 3)
  )
)

#       User      System    elapsed
#     145.47        0.09     152.48
```

RANGER SPEED

```
system.time(
  ames_ranger <- ranger(formula=Sale_Price ~ .,
    data      = ames_train,num.trees = 500,
    mtry      = floor(length(features) / 3))
)
```

```
##    user  system elapsed
##    8.05    0.05    3.03
```

The grid search

- To perform the grid search, we construct our grid of hyperparameters.
- We search across 96 different models with varying `mtry`, minimum node size, and sample size.

```
# hyperparameter grid search
hyper_grid <- expand.grid(
  mtry       = seq(20, 30, by = 2),
  node_size  = seq(3, 9, by = 2),
  sampe_size = c(.55, .632, .70, .80),
  OOB_RMSE   = 0
)

nrow(hyper_grid) # total number of combinations
```

```
## [1] 96
```

Loop - hyperparameter combination (I)

```
for(i in 1:nrow(hyper_grid)) {
  # train model
  model <- ranger(
    formula         = Sale_Price ~ .,
    data            = ames_train,
    num.trees       = 500,
    mtry            = hyper_grid$mtry[i],
    min.node.size   = hyper_grid$node_size[i],
    sample.fraction = hyper_grid$sampe_size[i],
    seed            = 123
  )
    # add OOB error to grid
  hyper_grid$OOB_RMSE[i] <- sqrt(model$prediction.error)
}
```

The results

```
hyper_grid %>%
  dplyr::arrange(OOB_RMSE) %>%
  head(10)
```

```
##    mtry node_size sampe_size OOB_RMSE
## 1    26         3        0.8 25404.60
## 2    28         3        0.8 25405.92
## 3    28         5        0.8 25459.46
## 4    26         5        0.8 25493.80
## 5    30         3        0.8 25528.26
## 6    22         3        0.7 25552.73
## 7    26         9        0.8 25554.31
## 8    28         7        0.8 25578.45
## 9    20         3        0.8 25581.23
## 10   24         3        0.8 25590.73
```

Loop - hyperparameter combination (I)

- We apply 500 trees since our previous example illustrated that 500 was plenty to achieve a stable error rate.
- We set the random number generator seed. This allows us to consistently sample the same observations for each sample size and make the impact of each change clearer.
- Our OOB RMSE ranges between 25000 - 26000.
- Our top 10 performing models all have RMSE values right around 25500 and the results show that models with slighly larger sample sizes (70-80 per cent) and deeper trees (3-5 observations in an terminal node) perform best.
- We get a full range of `mtry` values showing up in our top 10 - not over influential.

Hyperparameter grid search - categorical variables

- We use **one-hot encoding** for our categorical variables which produces 353 predictor variables versus the 80 we were using above.

```
# one-hot encode our categorical variables
(one_hot <- dummyVars(~ ., ames_train, fullRank = FALSE))
```

```
## Dummy Variable Object
##
## Formula: ~.
## 81 variables, 46 factors
## Variables and levels will be separated by '.'
## A less than full rank encoding is used
```

Make a dataframe of dummy variable object

```
ames_train_hot<-predict(one_hot,ames_train)%>%as.data.frame()
```

```
ames_train_hot[1:8,1:8]
```

```
##   MS_SubClass.One_Story_1946_and_Newer_All_Styles
## 1                                               1
## 2                                               1
## 3                                               1
## 4                                               0
## 5                                               0
## 6                                               0
## 7                                               0
## 8                                               1
##   MS_SubClass.One_Story_1945_and_Older
## 1                                    0
## 2                                    0
## 3                                    0
## 4                                    0
## 5                                    0
```

Hot encoding and hypergrid

```
# make ranger compatible names
names(ames_train_hot) <- make.names(names(ames_train_hot),
                                    allow_ = FALSE)
ames_train_hot <- predict(one_hot, ames_train) %>%
  as.data.frame()
# --> same as above but with increased mtry values
hyper_grid_2 <- expand.grid(
  mtry       = seq(50, 200, by = 25),
  node_size  = seq(3, 9, by = 2),
  sampe_size = c(.55, .632, .70, .80),
  OOB_RMSE  = 0
)
```

The best model

The best random forest model:

- retains columnar categorical variables
- `mtry` = 24,
- terminal node size of 5 observations
- sample size of 80%.

How to proceed

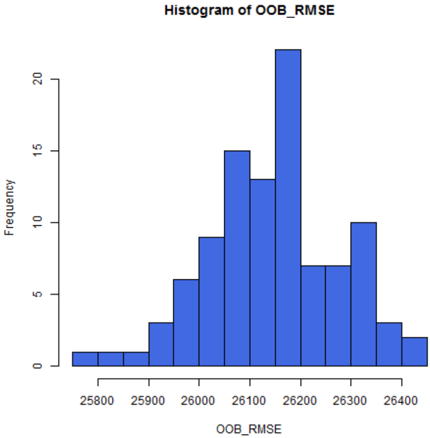
- repeat the model to get a better expectation of error rate.
- as expected error ranges between ~25,800-26,400

Random forests with ranger

```
OOB_RMSE <- vector(mode = "numeric", length = 100)

for(i in seq_along(OOB_RMSE)) {

  optimal_ranger <- ranger(
    formula         = Sale_Price ~ .,
    data            = ames_train,
    num.trees       = 500,
    mtry            = 24,
    min.node.size   = 5,
    sample.fraction = .8,
    importance      = 'impurity'
  )

  OOB_RMSE[i] <- sqrt(optimal_ranger$prediction.error)
}
```

A histogram of OOB RMSE

```
hist(OOB_RMSE, breaks = 20,col="royalblue")
```

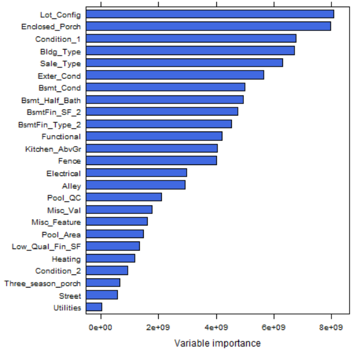


Variable importance

- We set `importance = 'impurity'`, which allows us to assess variable importance.
- **Variable importance** is measured by recording the decrease in MSE each time a variable is used as a node split in a tree.
- The remaining error left in predictive accuracy after a node split is known as node impurity and a variable that reduces this impurity is considered more imporant than those variables that do not.
- We accumulate the reduction in MSE for each variable across all the trees and the variable with the greatest accumulated impact is considered the more important, or impactful.
- We see that `Overall_Qual` has the greatest impact in reducing MSE across our trees, followed by `Gr_Liv_Area`, `Garage_Cars`, etc.

Plot the variable importance

```
varimp_ranger <- optimal_ranger$variable.importance
lattice::barchart(sort(varimp_ranger)[1:25],col="royalblue")
```



Predicting

- With the preferred model we can use the traditional predict function to make predictions on a new data set.
- We can use this for all our model types (`randomForest` and `ranger`); although the outputs differ slightly.

```
# randomForest
pred_randomForest <- predict(ames_randomForest, ames_test)
head(pred_randomForest)
```

```
##        1        2        3        4        5        6
## 113543.1 185556.4 259258.1 190943.9 179071.0 480952.3
```

```
# ranger
pred_ranger <- predict(ames_ranger, ames_test)
head(pred_ranger$predictions)
```

```
## [1] 129258.1 186520.7 265628.2 197745.5 175517.6 392691.7
```

Summary - random forests

- Random forests provide a very powerful out-of-the-box algorithm that often has great predictive accuracy.
- Because of their more simplistic tuning nature and the fact that they require very little, if any, feature pre-processing they are often one of the first go-to algorithms when facing a predictive modeling problem.

Advantages & Disadvantages

Advantages - random forrests

- Typically have very good performance
- Remarkably good "out-of-the box" - very little tuning required
- Built-in validation set - don't need to sacrifice data for extra validation
- No pre-processing required
- Robust to outliers

Disadvantages - random forrests

- Can become slow on large data sets
- Although accurate, often cannot compete with advanced boosting algorithms
- Less interpretable

Links

These slides are mainly based on

- A UC Business Analytics R Programming Guide - section **random forests**
- and on the **chapter on random forests** in the e-book of Brad Boehmke and Brandon Greenwell - Hands-on Machine Learning with R
- **Rpubs tutorial** - random forests
- Random Forests in R
- Boston Dataset-Tree Family Part-1