Model 1 Ensemble Classification Model (RANDOM FOREST)

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Preliminaries To avoid errors in laoding the dataset

Load Packages

```
##
## Attaching package: 'dplyr'

## The following objects are masked from 'package:stats':
##
##     filter, lag

## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union

## Warning: package 'ggplot2' was built under R version 4.2.2

## -- Attaching packages --------------------------------------- tidyverse 1.3.2 --

## v tibble  3.1.8     v stringr 1.5.0
## v tidyr   1.2.1     v forcats 0.5.2
## v purrr   0.3.5

## Warning: package 'stringr' was built under R version 4.2.2

## -- Conflicts ------------------------------------------ tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()

## Warning: package 'rsample' was built under R version 4.2.2

## Warning: package 'bestNormalize' was built under R version 4.2.2

##
## Attaching package: 'gridExtra'
##
## The following object is masked from 'package:dplyr':
##
##     combine

## Warning: package 'factoextra' was built under R version 4.2.2

## Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
##
## ----------------------------------------------------------------------
##
```

```
## Your next step is to start H2O:
##     > h2o.init()
##
## For H2O package documentation, ask for help:
##     > ??h2o
##
## After starting H2O, you can use the Web UI at http://localhost:54321
## For more information visit https://docs.h2o.ai
##
## ----------------------------------------------------------------------
##
##
## Attaching package: 'h2o'
##
## The following objects are masked from 'package:stats':
##
##     cor, sd, var
##
## The following objects are masked from 'package:base':
##
##     %*%, %in%, &&, ||, apply, as.factor, as.numeric, colnames,
##     colnames<-, ifelse, is.character, is.factor, is.numeric, log,
##     log10, log1p, log2, round, signif, trunc
##
## H2O is not running yet, starting it now...
##
## Note:  In case of errors look at the following log files:
##     C:\Users\c0set\AppData\Local\Temp\RtmpUViVex\file25d8546a33/h2o_c0set_started_from_r.out
##     C:\Users\c0set\AppData\Local\Temp\RtmpUViVex\file25d813e827c3/h2o_c0set_started_from_r.err
##
##
## Starting H2O JVM and connecting: . Connection successful!
##
## R is connected to the H2O cluster:
##     H2O cluster uptime:         5 seconds 242 milliseconds
##     H2O cluster timezone:       Asia/Taipei
##     H2O data parsing timezone:  UTC
##     H2O cluster version:        3.38.0.1
##     H2O cluster version age:    2 months and 27 days
##     H2O cluster name:           H2O_started_from_R_c0set_qmn693
##     H2O cluster total nodes:    1
##     H2O cluster total memory:   1.75 GB
##     H2O cluster total cores:    4
##     H2O cluster allowed cores:  4
##     H2O cluster healthy:        TRUE
##     H2O Connection ip:          localhost
##     H2O Connection port:        54321
##     H2O Connection proxy:       NA
##     H2O Internal Security:      FALSE
##     R Version:                  R version 4.2.1 (2022-06-23 ucrt)
```

Pre-processing of Data

Importing of Dataset

```
radiomicsdf<- read_csv("radiomics_completedata.csv")
```

```
## Rows: 197 Columns: 431
## -- Column specification --------------------------------------------------------
## Delimiter: ","
## chr   (1): Institution
## dbl (430): Failure.binary, Failure, Entropy_cooc.W.ADC, GLNU_align.H.PET, Mi...
##
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

```
#View(radiomicsdf)
head(radiomicsdf)
```

```
## # A tibble: 6 x 431
##   Institution Failure.~1 Failure Entro~2 GLNU_~3 Min_h~4 Max_h~5 Mean_~6 Varia~7
##   <chr>            <dbl>   <dbl>   <dbl>   <dbl>   <dbl>   <dbl>   <dbl>   <dbl>
## 1 A                    0   49.3     12.9    46.3    6.25   17.8     9.78   6.81
## 2 A                    1   12.6     12.2    27.5   11.0    26.5    15.4   12.9
## 3 A                    0   79.8     12.8    90.2    2.78    6.88    4.30   0.923
## 4 A                    1   17.9     13.5   326.     6.30   22.0    10.3    6.65
## 5 A                    0   39.6     12.6    89.6    3.58    7.92    4.45   0.572
## 6 A                    1    4.77    13.2   102.     2.60    6.21    3.77   0.615
## # ... with 422 more variables: Standard_Deviation_hist.PET <dbl>,
## #   Skewness_hist.PET <dbl>, Kurtosis_hist.PET <dbl>, Energy_hist.PET <dbl>,
## #   Entropy_hist.PET <dbl>, AUC_hist.PET <dbl>, H_suv.PET <dbl>,
## #   Volume.PET <dbl>, X3D_surface.PET <dbl>, ratio_3ds_vol.PET <dbl>,
## #   ratio_3ds_vol_norm.PET <dbl>, irregularity.PET <dbl>,
## #   tumor_length.PET <dbl>, Compactness_v1.PET <dbl>, Compactness_v2.PET <dbl>,
## #   Spherical_disproportion.PET <dbl>, Sphericity.PET <dbl>, ...
```

Checking for NULL and missing values

The result for checking null and missing values is 0 using *sum(is.n())*. Thus, there is no null and missing values

```
sum(is.na(radiomicsdf))
```

```
## [1] 0
```

Checking of Normality for the given dataset

```
radiomicsdfs=radiomicsdf%>%select_if(is.numeric)
radiomicsdfs=radiomicsdfs[,-c(1,2)]
radiomicsdf2=apply(radiomicsdfs,2,function(x){ks.test(x,"pnorm")})
```

Convert a list to vector

To have the list of p-value of all variables, the *unlist()* function is used and convert a list to vector.

```
KS_list=unlist(lapply(radiomicsdf2, function(x) x$p.value))
```

Checking for normality and non-normality of the given dataset

```
sum(KS_list<0.05) # not normally distributed
```

```
## [1] 428
```

```
sum(KS_list>0.05) # normally distributed
```

```
## [1] 0
```

[1] 428

[1] 1

Thus, we have 428 variables that are not normally distributed and Entropy_cooc.W.ADC is normally distributed.

Checking of variable with a maximum value

```
which.max(KS_list)
```

```
## Kurtosis_hist.PET
##                 9
```

CHECKING FOR THEN NORMALITY OF THE DATA

Check for normality, if not, normalized the data. Note that we used *Shapiro-Wilk's Test* to check the normality of the dataset

```
temdt=radiomicsdf[,c(3,5:length(names(radiomicsdf)))]

temdt=apply(temdt,2,orderNorm)
temdt=lapply(temdt, function(x) x$x.t)
temdt=temdt%>%as.data.frame()
test=apply(temdt,2,shapiro.test)
test=unlist(lapply(test, function(x) x$p.value))
```

```
sum(test>0.05) # not normally distributed
```

```
## [1] 428
```

```
sum(test<0.05) # not normally distributed
```

```
## [1] 0
```

#[1] 0 #[1] 428

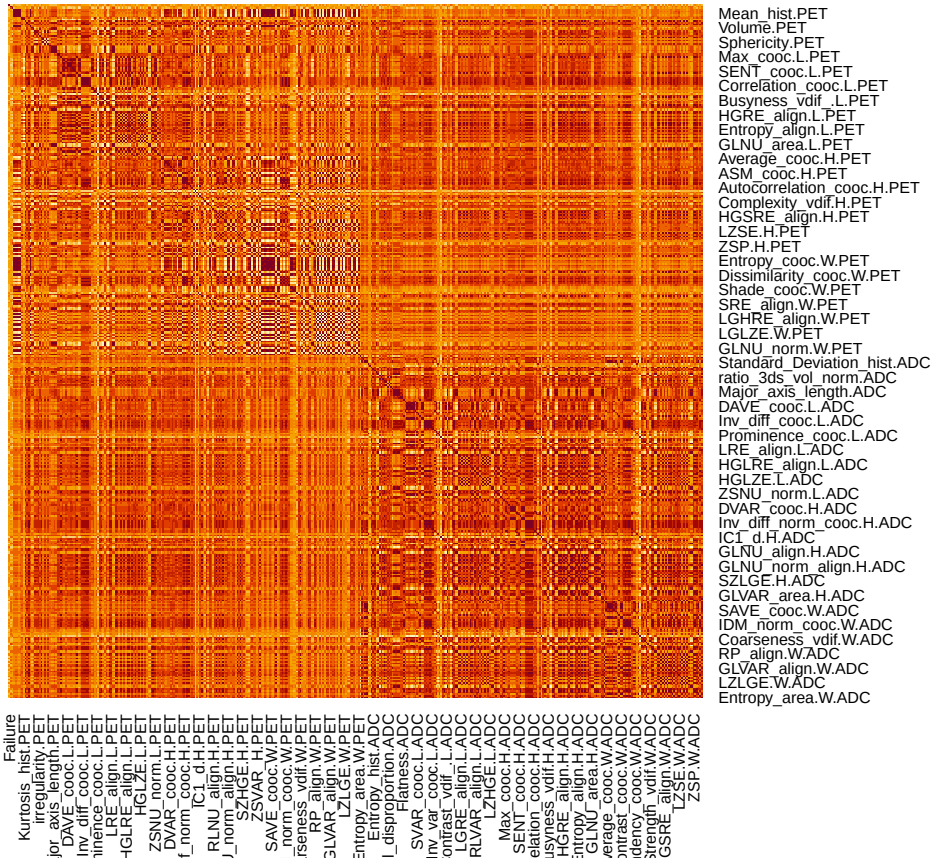
Thus, base on the result above our data is normally distributed.

The normalize dataset

```
radiomicsdf[,c(3,5:length(names(radiomicsdf)))]=temdt
```

CORRELATION OF THE WHOLE DATASET EXCEPT THE CATEGORICAL VARIABLES

```
CorMatrix=cor(radiomicsdf[,-c(1,2)])
heatmap(CorMatrix,Rowv=NA,Colv=NA,scale="none",revC = T)
```



SPLITTING THE DATA INTO TRAINING DATA (80%) AND TESTING DATA (20%)

```
radiomicsdf$Institution=as.factor(radiomicsdf$Institution)
radiomicsdf$Failure.binary=as.factor(radiomicsdf$Failure.binary)
```

```
splitter <- sample(1:nrow(radiomicsdf), round(nrow(radiomicsdf) * 0.8))
traindt <- radiomicsdf[splitter, ]
testdt  <- radiomicsdf[-splitter, ]
```

MODEL 1 RANDOM FOREST

Random Forest in R Programming is an ensemble of decision trees. It builds and combines multiple decision trees to get more accurate predictions. It's a non-linear classification algorithm

```
# Helper packages
library(ROCR)
library(pROC)
```

```
## Type 'citation("pROC")' for a citation.
```

```
##
## Attaching package: 'pROC'
```

```
## The following object is masked from 'package:h2o':
##
##     var
```

```
## The following objects are masked from 'package:stats':
##
##     cov, smooth, var
```

```
# Modeling packages
library(ranger)   # a c++ implementation of random forest
library(h2o)      # a java-based implementation of random forest
h2o.init()
```

```
##  Connection successful!
##
## R is connected to the H2O cluster:
##     H2O cluster uptime:         13 seconds 573 milliseconds
##     H2O cluster timezone:       Asia/Taipei
##     H2O data parsing timezone:  UTC
##     H2O cluster version:        3.38.0.1
##     H2O cluster version age:    2 months and 27 days
##     H2O cluster name:           H2O_started_from_R_c0set_qmn693
##     H2O cluster total nodes:    1
##     H2O cluster total memory:   1.75 GB
##     H2O cluster total cores:    4
##     H2O cluster allowed cores:  4
##     H2O cluster healthy:        TRUE
##     H2O Connection ip:          localhost
##     H2O Connection port:        54321
##     H2O Connection proxy:       NA
##     H2O Internal Security:      FALSE
##     R Version:                  R version 4.2.1 (2022-06-23 ucrt)
```

LOAD THE REPROCESSED DATASET

Note that we converted the reprocessed dataset into *.csv*. Hence, this dataset we used for the entire project named *normalRad.csv* ## Splitting of the normalized dataset

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

radiomicsdt<- read_csv("normalRad.csv")
```

```
## Rows: 197 Columns: 431
## -- Column specification --------------------------------------------------------
## Delimiter: ","
## chr   (1): Institution
## dbl (430): Failure.binary, Failure, Entropy_cooc.W.ADC, GLNU_align.H.PET, Mi...
```

```
##
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

```
radiomicsdt$Failure.binary=as.factor(radiomicsdt$Failure.binary)

split <- initial_split(radiomicsdt, strata = "Failure.binary")
traindt <- training(split)
testdt <- testing(split)

# number of features
no.features <- length(setdiff(names(traindt), "Failure.binary"))
```

Training of random forest model

```
# train a default random forest model
randomforest1 <- ranger(
  Failure.binary ~ .,
  data = traindt,
  mtry = floor(no.features / 3),
  respect.unordered.factors = "order",
  seed = 123
)
```

RMSE and hypergrid grid

```
# get OOB RMSE
(default_rmse <- sqrt(randomforest1$prediction.error))
```

```
## [1] 0.340068
```

```
# create hyperparameter grid
hyper_grid <- expand.grid(
  mtry = floor(no.features * c(.05, .15, .25, .333, .4)),
  min.node.size = c(1, 3, 5, 10),
  replace = c(TRUE, FALSE),
  sample.fraction = c(.5, .63, .8),
  rmse = NA
)

# execute full cartesian grid search
for(i in seq_len(nrow(hyper_grid))) {
  # fit model for ith hyperparameter combination
  fit <- ranger(
    formula         = Failure.binary ~ .,
    data            = traindt,
    num.trees       = no.features * 10,
    mtry            = hyper_grid$mtry[i],
    min.node.size   = hyper_grid$min.node.size[i],
    replace         = hyper_grid$replace[i],
    sample.fraction = hyper_grid$sample.fraction[i],
    verbose         = FALSE,
    seed            = 123,
    respect.unordered.factors = 'order',
  )
```

```
  # export OOB error
  hyper_grid$rmse[i] <- sqrt(fit$prediction.error)
}
```

Assess top 10 models

```
# assess top 10 models
hyper_grid %>%
  arrange(rmse) %>%
  mutate(perc_gain = (default_rmse - rmse) / default_rmse * 100) %>%
  head(10)
```

```
##    mtry min.node.size replace sample.fraction      rmse perc_gain
## 1   172             1    TRUE            0.50 0.3299144   2.98575
## 2   172             3    TRUE            0.50 0.3299144   2.98575
## 3   143            10    TRUE            0.50 0.3299144   2.98575
## 4   172            10    TRUE            0.50 0.3299144   2.98575
## 5   172            10   FALSE            0.50 0.3299144   2.98575
## 6   172            10    TRUE            0.63 0.3299144   2.98575
## 7   143             1    TRUE            0.50 0.3400680   0.00000
## 8   143             3    TRUE            0.50 0.3400680   0.00000
## 9   143             5    TRUE            0.50 0.3400680   0.00000
## 10  172             5    TRUE            0.50 0.3400680   0.00000
```

```
h2o.no_progress()
h2o.init(max_mem_size = "5g")
```

```
##  Connection successful!
##
## R is connected to the H2O cluster:
##     H2O cluster uptime:         5 minutes 10 seconds
##     H2O cluster timezone:       Asia/Taipei
##     H2O data parsing timezone:  UTC
##     H2O cluster version:        3.38.0.1
##     H2O cluster version age:    2 months and 27 days
##     H2O cluster name:           H2O_started_from_R_c0set_qmn693
##     H2O cluster total nodes:    1
##     H2O cluster total memory:   1.75 GB
##     H2O cluster total cores:    4
##     H2O cluster allowed cores:  4
##     H2O cluster healthy:        TRUE
##     H2O Connection ip:          localhost
##     H2O Connection port:        54321
##     H2O Connection proxy:       NA
##     H2O Internal Security:      FALSE
##     R Version:                  R version 4.2.1 (2022-06-23 ucrt)
```

Converting training dataset to h2o object

```
# converting training data to h2o object
train_h2o <- as.h2o(traindt)

# set the response column to Failure.binary
response <- "Failure.binary"
```

```r
# set the predictor names
predictors <- setdiff(colnames(traindt), response)

h2o_rf1 <- h2o.randomForest(
  x = predictors,
  y = response,
  training_frame = train_h2o,
  ntrees = no.features * 10,
  seed = 123
)
```

```
## Warning in .h2o.processResponseWarnings(res): Dropping bad and constant columns: [Institution].
```

```r
h2o_rf1
```

```
## Model Details:
## ==============
##
## H2OBinomialModel: drf
## Model ID:  DRF_model_R_1671212759374_1
## Model Summary:
##   number_of_trees number_of_internal_trees model_size_in_bytes min_depth
## 1            4300                     4300             1129975         4
##   max_depth mean_depth min_leaves max_leaves mean_leaves
## 1        13    6.76721          7         26    16.11860
##
##
## H2OBinomialMetrics: drf
## ** Reported on training data. **
## ** Metrics reported on Out-Of-Bag training samples **
##
## MSE:  0.1335695
## RMSE:  0.3654717
## LogLoss:  0.4232881
## Mean Per-Class Error:  0.1834021
## AUC:  0.8859794
## AUCPR:  0.7688701
## Gini:  0.7719588
## R^2:  0.4048858
##
## Confusion Matrix (vertical: actual; across: predicted) for F1-optimal threshold:
##         0  1    Error     Rate
## 0      75 22 0.226804   =22/97
## 1       7 43 0.140000    =7/50
## Totals 82 65 0.197279  =29/147
##
## Maximum Metrics: Maximum metrics at their respective thresholds
##                         metric threshold     value idx
## 1                       max f1  0.322825  0.747826  64
## 2                       max f2  0.230769  0.842105  84
## 3                 max f0point5  0.683418  0.760870  21
## 4                 max accuracy  0.436593  0.823129  43
## 5                max precision  0.683418  0.954545  21
## 6                   max recall  0.132872  1.000000 114
```

```
## 7              max specificity  0.872517  0.989691   0
## 8             max absolute_mcc  0.322825  0.604012  64
## 9   max min_per_class_accuracy  0.369259  0.793814  59
## 10 max mean_per_class_accuracy  0.322825  0.816598  64
## 11                     max tns  0.872517 96.000000   0
## 12                     max fns  0.872517 50.000000   0
## 13                     max fps  0.031170 97.000000 146
## 14                     max tps  0.132872 50.000000 114
## 15                     max tnr  0.872517  0.989691   0
## 16                     max fnr  0.872517  1.000000   0
## 17                     max fpr  0.031170  1.000000 146
## 18                     max tpr  0.132872  1.000000 114
##
## Gains/Lift Table: Extract with `h2o.gainsLift(<model>, <data>)` or `h2o.gainsLift(<model>, valid=<T/
```

Hyperparameter grid

```
# hyperparameter grid
hyper_grid <- list(
  mtries = floor(no.features * c(.05, .15, .25, .333, .4)),
  min_rows = c(1, 3, 5, 10),
  max_depth = c(10, 20, 30),
  sample_rate = c(.55, .632, .70, .80)
)

# random grid search strategy
search_criteria <- list(
  strategy = "RandomDiscrete",
  stopping_metric = "mse",
  stopping_tolerance = 0.001,   # stop if improvement is < 0.1%
  stopping_rounds = 10,         # over the last 10 models
  max_runtime_secs = 60*5      # or stop search after 5 min.
)
```

Perform grid search

```
# perform grid search
random_grid <- h2o.grid(
  algorithm = "randomForest",
  grid_id = "rf_random_grid",
  x = predictors,
  y = response,
  training_frame = train_h2o,
  hyper_params = hyper_grid,
  ntrees = no.features * 10,
  seed = 123,
  stopping_metric = "RMSE",
  stopping_rounds = 10,           # stop if last 10 trees added
  stopping_tolerance = 0.005,     # don't improve RMSE by 0.5%
  search_criteria = search_criteria
)
```

Collect results and model performance

```r
# collect the results and sort by our model performance metric
# of choice
random_grid_perf <- h2o.getGrid(
  grid_id = "rf_random_grid",
  sort_by = "mse",
  decreasing = FALSE
)
random_grid_perf
```

```
## H2O Grid Details
## ================
##
## Grid ID: rf_random_grid
## Used hyper parameters:
##   -  max_depth
##   -  min_rows
##   -  mtries
##   -  sample_rate
## Number of models: 240
## Number of failed models: 0
##
## Hyper-Parameter Search Summary: ordered by increasing mse
##   max_depth min_rows    mtries sample_rate                model_ids     mse
## 1  30.00000  1.00000 143.00000     0.80000 rf_random_grid_model_188 0.08344
## 2  20.00000  1.00000 143.00000     0.80000 rf_random_grid_model_206 0.08344
## 3  10.00000  1.00000 143.00000     0.80000 rf_random_grid_model_215 0.08344
## 4  10.00000  3.00000 143.00000     0.63200 rf_random_grid_model_133 0.08621
## 5  30.00000  3.00000 143.00000     0.63200  rf_random_grid_model_19 0.08621
##
## ---
##     max_depth min_rows   mtries sample_rate                model_ids     mse
## 235  20.00000 10.00000 21.00000     0.80000 rf_random_grid_model_235 0.15089
## 236  30.00000 10.00000 21.00000     0.80000   rf_random_grid_model_3 0.15089
## 237  10.00000 10.00000 21.00000     0.80000  rf_random_grid_model_52 0.15089
## 238  20.00000  1.00000 21.00000     0.80000  rf_random_grid_model_30 0.15812
## 239  30.00000  1.00000 21.00000     0.80000  rf_random_grid_model_98 0.15812
## 240  10.00000  1.00000 21.00000     0.80000 rf_random_grid_model_149 0.15950
```

Model with impurity-based variable importance

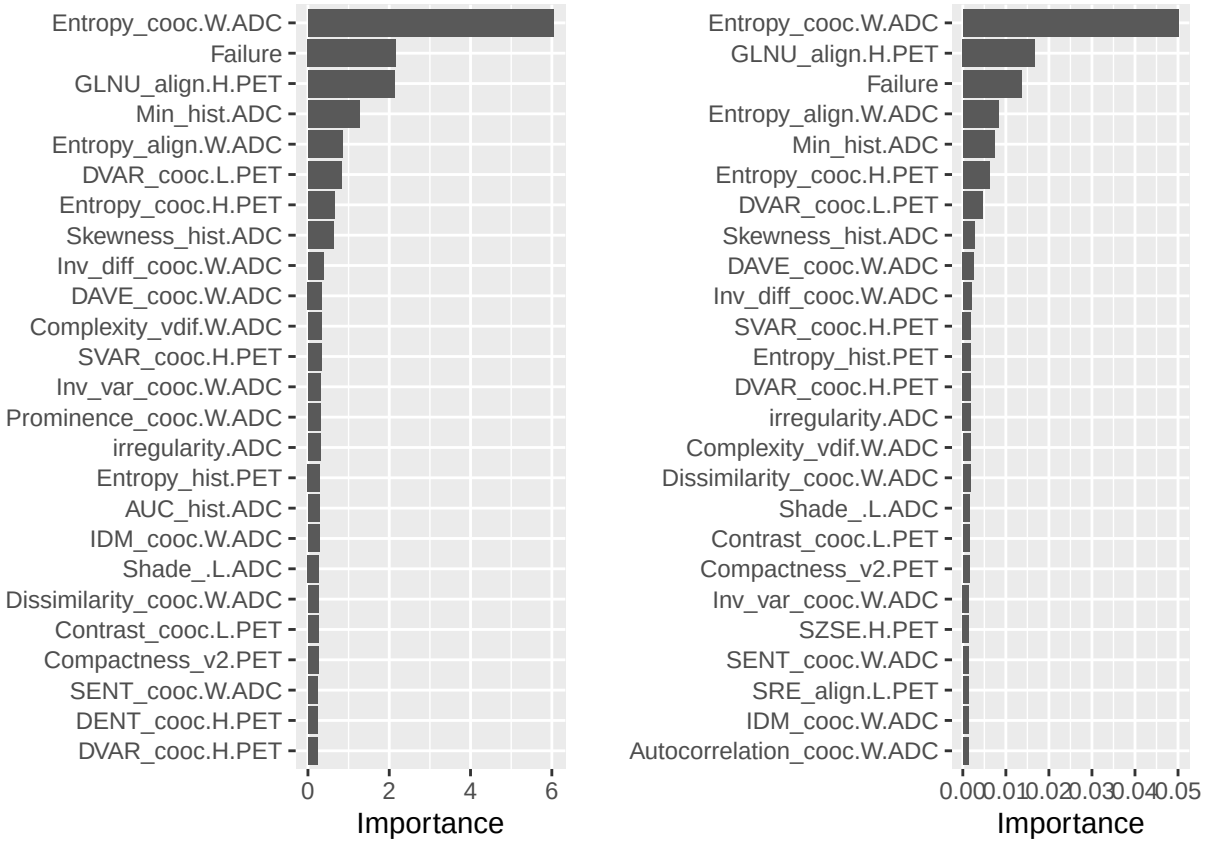
```r
# re-run model with impurity-based variable importance
rf_impurity <- ranger(
  formula = Failure.binary ~ .,
  data = traindt,
  num.trees = 2000,
  mtry = 32,
  min.node.size = 1,
  sample.fraction = .80,
  replace = FALSE,
  importance = "impurity",
  respect.unordered.factors = "order",
  verbose = FALSE,
  seed  = 123
)
```

Permutation-based variable importance

```
# re-run model with permutation-based variable importance
rf_permutation <- ranger(
  formula = Failure.binary ~ .,
  data = traindt,
  num.trees = 2000,
  mtry = 32,
  min.node.size = 1,
  sample.fraction = .80,
  replace = FALSE,
  importance = "permutation",
  respect.unordered.factors = "order",
  verbose = FALSE,
  seed  = 123
)
```

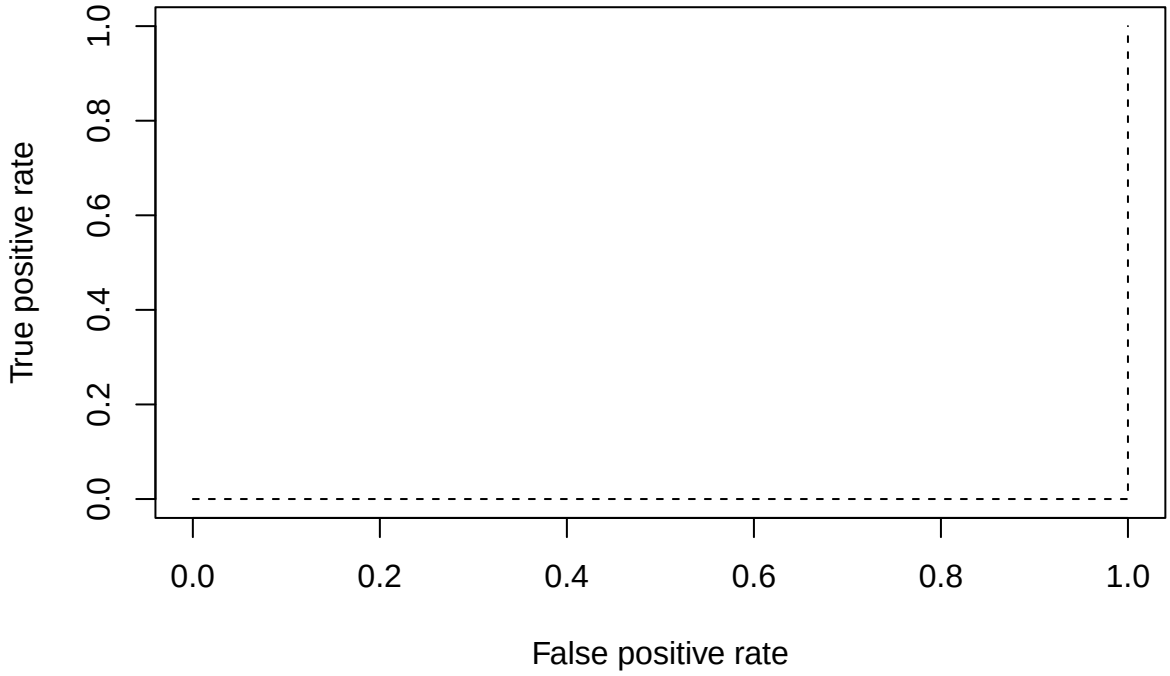
Plotting of important varriables

```
p1 <- vip::vip(rf_impurity, num_features = 25, bar = FALSE)
p2 <- vip::vip(rf_permutation, num_features = 25, bar = FALSE)

gridExtra::grid.arrange(p1, p2, nrow = 1)
```



Compute probabilities and plotting of AUC

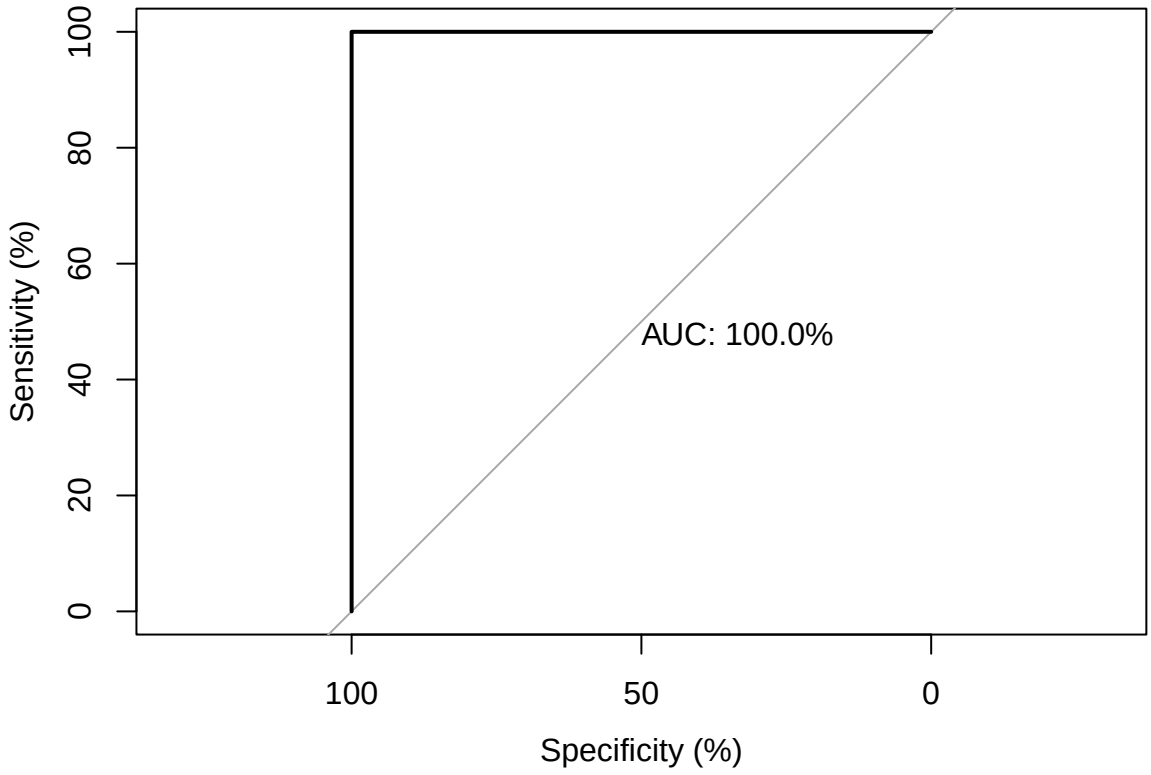
```
# Compute predicted probabilities on training data
m1_prob <- predict(h2o_rf1, train_h2o, type = "prob")
m1_prob=as.data.frame(m1_prob)[,2]
train_h2o=as.data.frame(train_h2o)
# Compute AUC metrics for cv_model1,2 and 3
perf1 <- prediction(m1_prob,train_h2o$Failure.binary) %>%
  performance(measure = "tpr", x.measure = "fpr")


# Plot ROC curves for cv_model1,2 and 3
plot(perf1, col = "black", lty = 2)
```




```
# ROC plot for training data
roc( train_h2o$Failure.binary ~ m1_prob, plot=TRUE, legacy.axes=FALSE,
    percent=TRUE, col="black", lwd=2, print.auc=TRUE)
```

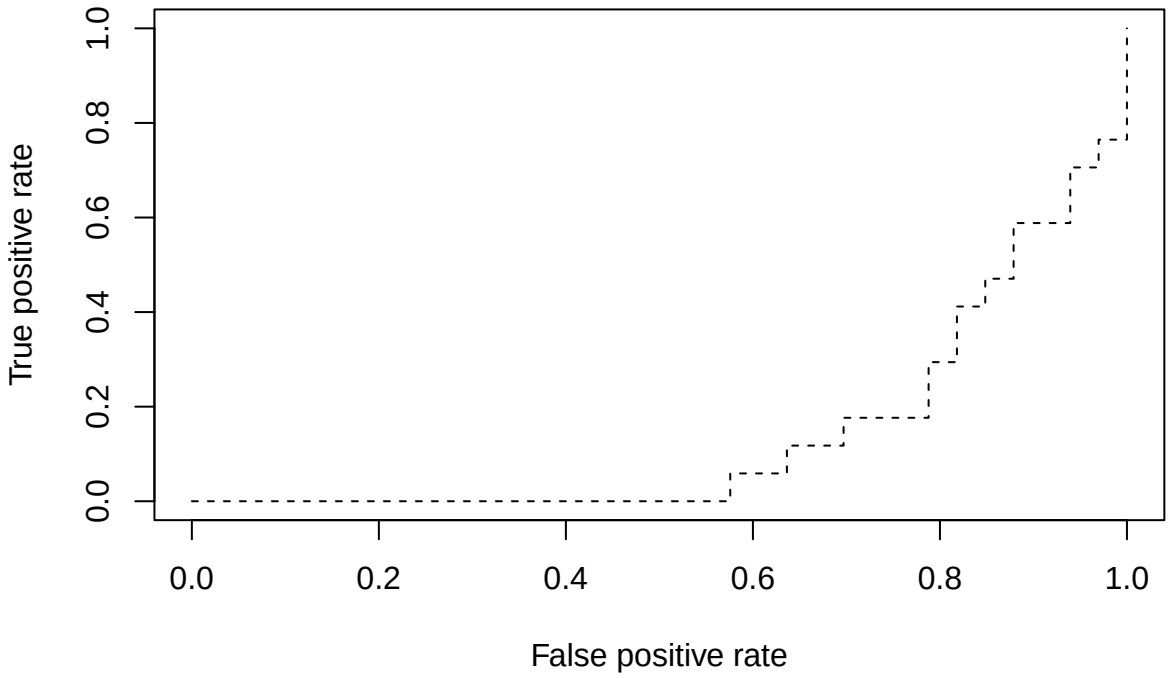
```
## Setting levels: control = 0, case = 1
```

```
## Setting direction: controls > cases
```



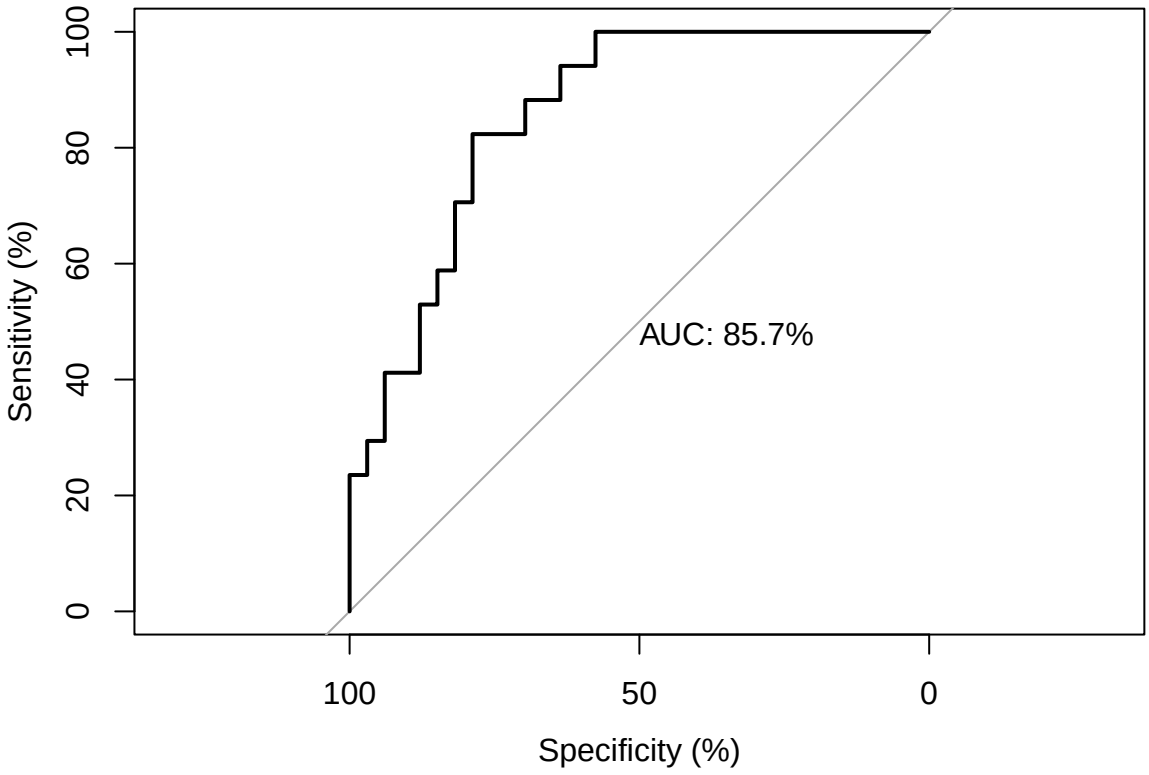

```
##
## Call:
## roc.formula(formula = train_h2o$Failure.binary ~ m1_prob, plot = TRUE,     legacy.axes = FALSE, perc
##
## Data: m1_prob in 97 controls (train_h2o$Failure.binary 0) > 50 cases (train_h2o$Failure.binary 1).
## Area under the curve: 100%
```

```
# #Feature Interpretation
# vip(cv_model3, num_features = 20)

# Compute predicted probabilities on training data
test_h2o=as.h2o(testdt)

m2_prob <- predict(h2o_rf1, test_h2o, type = "prob")

m2_prob=as.data.frame(m2_prob)[,2]

test_h2o=as.data.frame(test_h2o)

# Compute AUC metrics for cv_model1,2 and 3
perf2 <- prediction(m2_prob,test_h2o$Failure.binary) %>%
  performance(measure = "tpr", x.measure = "fpr")


# Plot ROC curves for cv_model1,2 and 3
plot(perf2, col = "black", lty = 2)
```




```
# ROC plot for training data
roc( test_h2o$Failure.binary ~ m2_prob, plot=TRUE, legacy.axes=FALSE,
    percent=TRUE, col="black", lwd=2, print.auc=TRUE)
```

```
## Setting levels: control = 0, case = 1
## Setting direction: controls > cases
```




```
##
## Call:
## roc.formula(formula = test_h2o$Failure.binary ~ m2_prob, plot = TRUE,     legacy.axes = FALSE, percen
##
## Data: m2_prob in 33 controls (test_h2o$Failure.binary 0) > 17 cases (test_h2o$Failure.binary 1).
## Area under the curve: 85.74%
```