Minicourse II
Introduction to Statistical Learning with tidymodels

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Day 1

- Intro to statistical learning
- Assessing Model Accuracy
- Classification and regression decision trees.
- Focused on CART algorithm
- Introduction to `tidymodels`
- Example with `tidymodels`

Day 2

- Resampling, Cross validation
- Ensemble methods
- Random Forest
- Hyperprameter tuning and model comparison
- How to do all with `tidymodels`

Working with tidymodel

GitHub repo with slides and data

```
library(tidyverse)
library(tidymodels)
library(here)
data <- read_csv(here("apt_redu.csv"))
```

Working with tidymodels

Fit a decision tree (classification) for Montevideo apparment price in Pocitos neigborhood

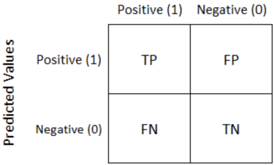
```
#Transform the response in a two class vble
new_data <- data %>%
  mutate(lpreciom2_c = as.factor(
    case_when(lpreciom2< mean(lpreciom2)~'low',
                        lpreciom2 >= mean(lpreciom2) ~ 'high'))) %>%
                          select(-lpreciom2,-long)
#Split the data

set.seed(2023)
data_split_c <- initial_split(new_data)

data_train_c <- training(data_split_c)
data_test_c <- testing(data_split_c)
```

```
#parsnip pkg
# Pick a model,  Set the engine and set mod
 tree_mod_cl<- decision_tree() %>%
   set_engine("rpart") %>%
    set_mode("classification")

## it the model with the training data set
tree_fit_cl <- tree_mod_cl %>%
        fit(lpreciom2_c ~ ., data = data_train_c)

# Get the performance in the training set
augment(tree_fit_cl, new_data = data_test_c ) %>%
accuracy(truth = lpreciom2_c , estimate = .pred_class)
```

```
## # A tibble: 1 x 3
##   .metric  .estimator .estimate
##   <chr>    <chr>          <dbl>
## 1 accuracy binary         0.735
```

More accuracy measures for classification

Confusion matrix



		Positive (1)	Negative (0)
Predicted Values	Positive (1)	TP	FP
	Negative (0)	FN	TN

- Accuracy: $\frac{TP+TN}{Totalobs}$
- Error: $\frac{FP+FN}{Totalobs}$
- Sensitivity: $\frac{TP}{TP+FN}$ True positive
- Specificity: $\frac{TN}{TN+FP}$ True negative

Confusion matrix

```
# Get the performance in the training set
augment(tree_fit_cl, new_data = data_test_c ) %>%
  conf_mat(truth =lpreciom2_c , estimate = .pred_class)
```

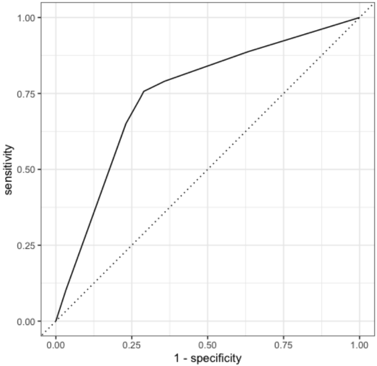
```
##           Truth
## Prediction high  low
##       high 1522  529
##       low   489 1298
```

ROC curve

- ROC curve (Receiver Operating Characteristic) it is a graphic that shows simultaneously the two types of accuracies (sensitivity and specificity) for all possible discrimination thresholds.
- Use to compare classification methods
- The area under the curve ROC is the AUC, closer to 1 implies better model fit

To generate a ROC curve, we need the predicted class probabilities for high and low, which is calculated augment
We can create the ROC curve with these values, using roc_curve() and then piping to the autoplot()

```
augment(tree_fit_cl, new_data = data_test_c) %>%
  roc_curve(truth = lpreciom2_c, .pred_high) %>%
  autoplot()
```


1.00
0.75
0.50
0.25
0.00
sensitivity
0.00
0.25
0.50
0.75
1.00
1 - specificity

AUC

```
augment(tree_fit_cl, new_data = data_test_c ) %>%
roc_auc(truth = lpreciom2_c, .pred_high)

## # A tibble: 1 x 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 roc_auc binary         0.747
```

Training and test approach

- We have mentioned in the first class the distinction between the test error rate and the training error and you should use the test set to evaluate the model

- Main idea is to use a different data set to train and evaluate the model

- Estimated the prediction error with training data underestimate the error.

Training and test approach

Dividing the data in trainig and test is simple to understand and implement but have some limitiations

- Sometimes we don't have enough data in test set to have a good test error estimation.
- The test error rate can be highly variable, depending on which observations are included in the training set and which observations are included in the test set

We will ses a resample method that overcome these issues

Resampling

Resampling methods are really important in modern statistics.

Idea: repeatedly drawing samples from a training set and refitting a model of interest on each sample in order to obtain additional information about the fitted model

- Generate (sub)-samples from the training data set.
- We can use them to evaluate statistical properties: bias, standard error, prediction error
- Select the tuning parameters based on resampling methods

We will see Cross-validation

Cross-validation is a very general approach that can be applied to almost any statistical learning method.

Cross-validation

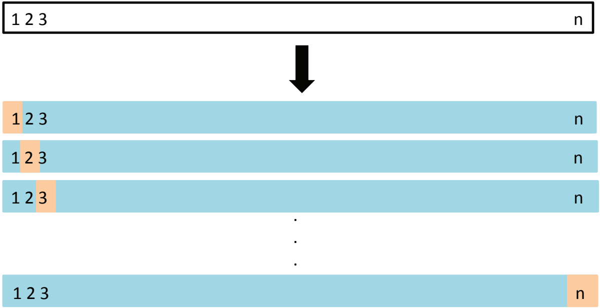
Resampling method that will be used to estimate the model predictive error

- Copmpare models and select the model with smaller error.
- Method for *tuning parameters*.

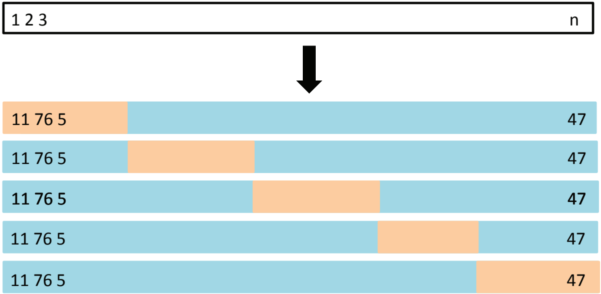
There are several ways to divide the data if we have n observations:

- We can use $n-1$ observations to estimate the model and 1 to predict and repeat this n times (Leave-one-out,LOO).
- k groups with $k < n$: estimate with $n-n/k$ and predict with n/k, repeat k times (k-fold CV).

Leave-One-Out Cross-Validation



Cross-validation, *k*fold



k-Fold Cross-Validation, MSE estimation

This process results in k estimates of the test error, $MSE_1, MSE_2, ..., MSE_k$. The k-fold CV estimate is computed by averaging these values,

$$CV_k(\hat{f}) = \frac{1}{k}\sum_{j=1}^{k} MSE_j$$

Cross-validation: hyperparameter tuning

If your model have additional parameters to tune: $\hat{f}(x, \alpha)$

- Get $CV(\hat{f}, \alpha)$ for different α values
- Select $\hat{\alpha}$ which minimizes $CV(\hat{f}, \alpha)$

tuning parameters with tidymodels

To use k-Fold Cross-Validation we will be using the tune package, and we need 3 things to get it working:

- A parsnip/workflow object with one or more arguments marked for tuning
- A vfold_cv rsample object of the cross-validation resamples,
- A tibble denoting the values of hyperparameter values to be explored.

Resampling with tidymodels

We already see how to use parsnip which can be used to define and fit the model Now we will explote workflow package to do CV.
The objective of an workflow() object is to encapsulate the major pieces of the modeling process

- using a workflow concept encourages good methodology since it is a single point of entry to the estimation components of a data analysis.
- It enables the user to better organize projects.

workflow() is a container object that aggregates information required to fit and predict from a model
Check library(help='workflows')

- workflow: Create a workflow
- add_model: Add a model to a workflow
- fit-workflow: Fit a workflow object
- add_formula: Add formula terms to a workflow
- predict-workflow:Predict from a workflow

```
tree_cl_wf <-
  workflow() %>%
  add_model(spec = tree_mod_cl) %>%
  add_formula(lpreciom2_c ~ .)

tree_cl_wf

## == Workflow ========================================================
## Preprocessor: Formula
## Model: decision_tree()
##
## -- Preprocessor ----------------------------------------------------
## lpreciom2_c ~ .
##
## -- Model -----------------------------------------------------------
## Decision Tree Model Specification (classification)
##
## Computational engine: rpart
```

10-fold CV with tidymodel

vfold_cv randomly splits the data into V groups of roughly equal size

```
set.seed(2023)
folds <- vfold_cv(data_train_c, v = 10)
folds

## #  10-fold cross-validation
## # A tibble: 10 x 2
##    splits               id
##    <list>               <chr>
##  1 <split [10360/1152]> Fold01
##  2 <split [10360/1152]> Fold02
##  3 <split [10361/1151]> Fold03
##  4 <split [10361/1151]> Fold04
##  5 <split [10361/1151]> Fold05
##  6 <split [10361/1151]> Fold06
##  7 <split [10361/1151]> Fold07
##  8 <split [10361/1151]> Fold08
##  9 <split [10361/1151]> Fold09
```

fit_rsamples from the package tune computes a set of performance metrics across one or more resamples.

```
tree_fit_rs <-
  tree_cl_wf %>% #classificcation tree workflow
  fit_resamples(folds) # compute metrics in across folds

tree_fit_rs

## # Resampling results
## # 10-fold cross-validation
## # A tibble: 10 x 4
##    splits               id     .metrics         .notes
##    <list>               <chr>  <list>           <list>
##  1 <split [10360/1152]> Fold01 <tibble [2 x 4]> <tibble [0 x 3]>
##  2 <split [10360/1152]> Fold02 <tibble [2 x 4]> <tibble [0 x 3]>
##  3 <split [10361/1151]> Fold03 <tibble [2 x 4]> <tibble [0 x 3]>
##  4 <split [10361/1151]> Fold04 <tibble [2 x 4]> <tibble [0 x 3]>
##  5 <split [10361/1151]> Fold05 <tibble [2 x 4]> <tibble [0 x 3]>
##  6 <split [10361/1151]> Fold06 <tibble [2 x 4]> <tibble [0 x 3]>
##  7 <split [10361/1151]> Fold07 <tibble [2 x 4]> <tibble [0 x 3]>
```

At the end of this process, there are 10 sets of performance statistics that were created on 10 data sets that were not used in the modeling process

The final resampling estimates for the model are the averages of the performance statistics replicates

By default in classificcation problemsaccuracy and roc_auc are computed

```
collect_metrics(tree_fit_rs )

## # A tibble: 2 x 6
##   .metric  .estimator  mean     n std_err .config
##   <chr>    <chr>      <dbl> <int>   <dbl> <chr>
## 1 accuracy binary     0.716    10 0.00373 Preprocessor1_Model1
## 2 roc_auc  binary     0.738    10 0.00469 Preprocessor1_Model1
```

Tuning cost_complexity

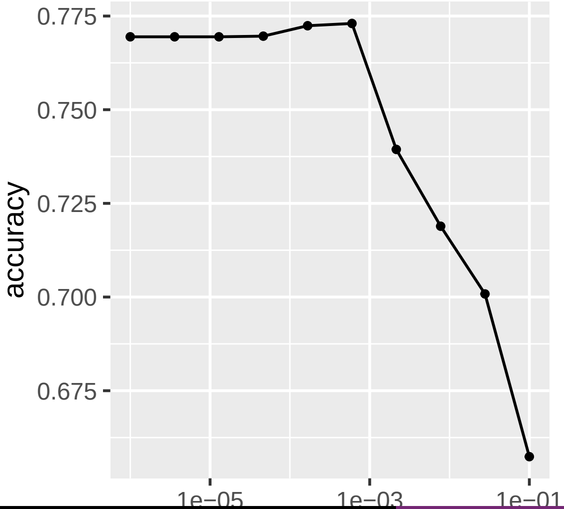
- Lets tune the cost_complexity of the decision tree to find a more optimal complexity.
- We use the tree_mod_cl object and use the set_args() function to specify that we want to tune cost_complexity.
- set_args can be used to modify the arguments of a model specification while

```
tree_cl_tunewf <-
  workflow() %>%
  add_model(spec = tree_mod_cl %>%
              set_args(cost_complexity = tune())) %>%
  add_formula(lpreciom2_c ~ .)
```

We need a resamples objects, we will use a k-fold cross-validation data set, and a grid of values to try. Only tuning 1 hyperparameter it is fine to stay with a regular grid.

```r
param_grid <- grid_regular(cost_complexity(range = c(-6, -1)),
                           levels = 10)

tune_res <- tune_grid(
  tree_cl_tunewf,
  resamples = folds,
  grid = param_grid,
  metrics = metric_set(accuracy))
```

```
autoplot(tune_res)
```



We can select the best performing value with select_best(), finalize the workflow by updating the value of cost_complexity and fit the model on the full training data set.

```
best_cp <- select_best(tune_res)

tree_cl_final <- finalize_workflow(tree_cl_tunewf, best_cp)


#takes a data split as an input, uses the split to generate
#the training and test sets for the final fitting and evaluation.

tree_cl_final_fit <-  last_fit(tree_cl_final,data_split_c )
```

```
fitted_wflow <- extract_workflow(tree_cl_final_fit)

collect_metrics(tree_cl_final_fit)%>% slice(1:5)

## # A tibble: 2 x 4
##   .metric  .estimator .estimate .config
##   <chr>    <chr>          <dbl> <chr>
## 1 accuracy binary         0.769 Preprocessor1_Model1
## 2 roc_auc  binary         0.814 Preprocessor1_Model1
```

Some tree disadvantages

:

- In general does not present good predictive performance if we compare with other methods
- Are not robust, small changes in data can cause big changes in final estimations.

There are methods that try to overcome those disadvantages. Main idea is to combine a lot of decision trees and get sustantial improvement in the predictive performance.

Ensemble methods

- Ensembles learning methods: combined multiple individual models trained independently to build a prediction model potentially better.
- Some well known examples of ensemble learning methods are, boosting (Schapire, R., 1990), bagging (Breiman,L., 1996) and random forest (Breiman, L., 2001) among others.
- Main differences between ensembles, type of individual models to be combined and the ways these individual models are combined.

Bagging

Bagging or bootstrap aggregation:

- Bagging main idea is to average noisy, approximately unbiased models to reduce the variance.
- Bagging, fits many trees to different bootstrap samples.
- Bootstrap samples: B random samples with replacement from the training data set with the same size.
- CART trees are *unestables*, small changes in training set can generate big changes in the final model .

Trees are **good** candidates to do *bagging*.

- capture complex interactions
- small bias (if are big enough)

Random forest

- Supervised ensemble lerning method, built on bagged trees(Breiman, L., 2021)
- Widely used (more than 106 thousand citations 2023).
- Can be used for regession or classification problems.
- For regression, Random Forest (RF) smoothes the estimate by averaging over a set of trees.

It is based on averaging a set of randomized trees.

Random Forest

Main concepts:

- Bootstrap aggregation (Breiman, L., (1996) and Breiman, L., et.al. (1996))
- Random feature selection (Amit. Y., and Geman, D., (1997) and Ho, T., (1998)) to individual classification trees for prediction.

Random forest

Problem context, $Y = f(X) + \varepsilon$, *RF*, if the response is quantitative f is estimated as follows:

$$\hat{f}_{rf}(x) = \frac{1}{B}\sum_{b} T(x, \Theta_b)$$

where $T(x, \theta_b)$ it is a *randomized* tree.

Θ_b contains **two** sources of randomness:

- trained with a bootstrap sample (same as *bagging*)
- random variable selection for each node partition

The idea is the same as bagging in terms of variance reduction and gets additional improvement based on the additional source of randomness incorporated.

Forest algorithm

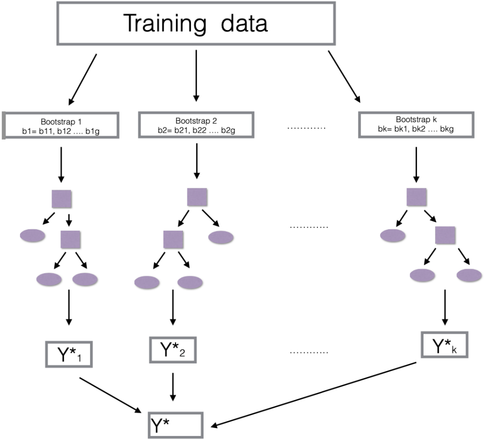
Get a set of randomized trees $\{T_b\}_1^B$. For $b \in 1, 2, \ldots, B$

1. Select a bootstrap sample Z^b with size N
2. With Z^b, fit the tree T_b,type CART with two modifications:
    - in each node, just m variables selected at random are used
    - let the tree grow to the end without pruning

Later:

- **Regression** $\hat{f}_{rf} = \frac{1}{B}\sum_{b=1}^{B} T(x, \theta_b)$
- **Clssification** $\hat{f}_{rf} = argmax_g \frac{1}{B}\sum_{b=1}^{B} I(T(x, \theta_b) = g)$ majority vote

RF diagram


Training data
Bootstrap 1
b1= b11, b12 .... b1g
Bootstrap 2
b2= b21, b22 .... b2g
Bootstrap k
bk= bk1, bk2 .... bkg
....
Y*1
Y*2
Y*k
Y*

Auxiliar parameters

Basic parameters: B, m leaf size.
Decreasing m reduces the correlation between pairs of trees and decreases the variance of the mean. But also each individual tree is worse.

Default values:

- Classification, default $\sqrt(p)$ and min node size is 1.
- Regression, default m value is $p/3$ and min node size is 5
- B value depends on the computational implementation.

OOB sample

- Each bootstrap sample has an associate data set which got *out of bag*, OOB_b.
- For each observation $z_i = (x_i, y_i)$, we can do a prediction using **just** trees T_b where $z_i \in OOB_b$.

Define:

$$errOOB = \frac{1}{N}\sum_i (\hat{y}_i^{oob} - y_i)^2$$

The estimated OOB error is almost identical to the error estimated by a k-fold cross-validation.

Overfitting

- When the number of variables is big but a small number of them are relevant, RF is probable to not fit very well if the selected m is small.
- In each partition there will be small chances to select some relevant variables.
- RF is promoted as a non-overfitting method, increasing B does not cause overfitting

Variable importance

Tell us how important a variable is for the predictive model.
In each tree partition, the improvement in the partition criteria is the importance measure for that variable and the value is accumulated across all the trees in the forest.
RF uses the OOB observations for another importance variable measure which allows to measure the strength of each variable to predict (permuted importance variable)

Permuted importance measure

For each tree $T_b(x, \theta_b)$an error measure is compute with OOB_b observations

$$VI_j = \frac{1}{B} \sum_b erOOB_b^* - erOOB_b$$

$erOOB_b^*$ it is the error in $T_b(x, \theta_b)$ after randomly permuting X_j values.

- X_j is an important variable if the model error gets larger when the variable is permuted

Random Forest with tidymodels

```
rf_spec <-
  rand_forest() %>%
  set_engine("ranger", importance = "permutation") %>%
  set_mode("classification")

rf_fit <- fit(rf_spec, lpreciom2_c ~ ., data = data_train_c)
rf_fit
```

```
## parsnip model object
##
## Ranger result
##
## Call:
##  ranger::ranger(x = maybe_data_frame(x), y = y, importance = ~"permu
##
## Type:                             Probability estimation
## Number of trees:                  500
## Sample size:                      11512
```

Training vs test accuracy

```
augment(rf_fit, new_data = data_train_c) %>%
accuracy(truth = lpreciom2_c, estimate = .pred_class)
```

```
## # A tibble: 1 x 3
##   .metric  .estimator .estimate
##   <chr>    <chr>          <dbl>
## 1 accuracy binary         0.930
```

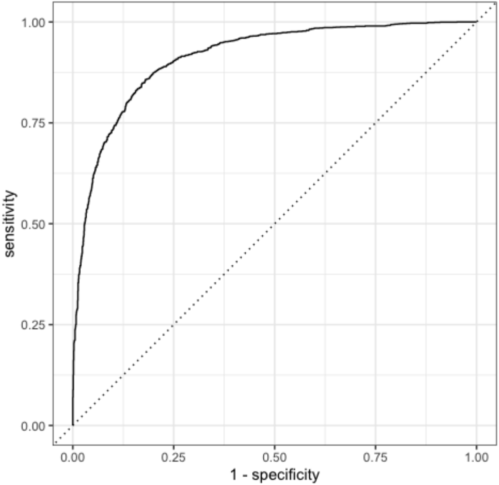
```
augment(rf_fit, new_data = data_test_c) %>%
accuracy(truth = lpreciom2_c, estimate = .pred_class)
```

```
## # A tibble: 1 x 3
##   .metric  .estimator .estimate
##   <chr>    <chr>          <dbl>
## 1 accuracy binary         0.837
```

```r
augment(rf_fit, new_data = data_test_c) %>%
  roc_auc(truth = lpreciom2_c, .pred_high)
```

```
## # A tibble: 1 x 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 roc_auc binary         0.913
```

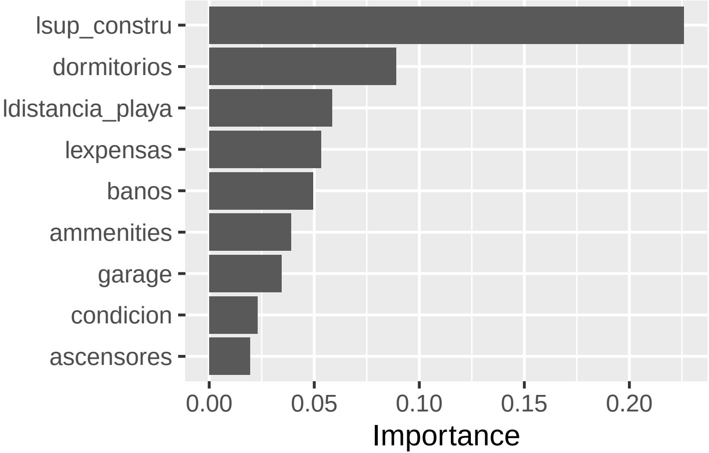
```r
augment(rf_fit, new_data = data_test_c) %>%
  roc_curve(truth = lpreciom2_c, .pred_high) %>%
  autoplot()
```


1.00
0.75
0.50
0.25
0.00
sensitivity
0.00
0.25
0.50
0.75
1.00
1 - specificity

Variable importance with vip

```r
library(vip)
vip(rf_fit)
```

Variable importance with vip



Tuning and model comparison with tidymodels

We want to compare tree different tuned models

```
library(baguette)

apt_folds <- vfold_cv(data_train_c, repeats = 5, v = 5) # 5-fold-CV-5reps
#1) Set models (CART, Bagging and Random Forest)

cart_apt <-
  decision_tree(cost_complexity = tune()) %>%
  set_engine("rpart") %>%
  set_mode("classification")

bag_cart_apt <- bag_tree(cost_complexity = tune(),
                         class_cost = tune() ) %>%
  set_mode("classification")

rf_apt <-
  rand_forest(mtry = tune(), min_n = tune(), trees = 1000) %>%
  set_engine("ranger") %>%
  set_mode("classification")
```

Workflow

```
#define for all the models variables to be use
model_vars <-
  workflow_variables(outcomes = lpreciom2_c ,
                     predictors = everything())

#Generate a set of workflow objects from preprocessing
#and model objects
wkf <-
  workflow_set(
    preproc = list(simple = model_vars), #A list with preproc.obj

    models = list(CART = cart_apt, bagging = bag_cart_apt, RF = rf_apt)
  )

wkf
```

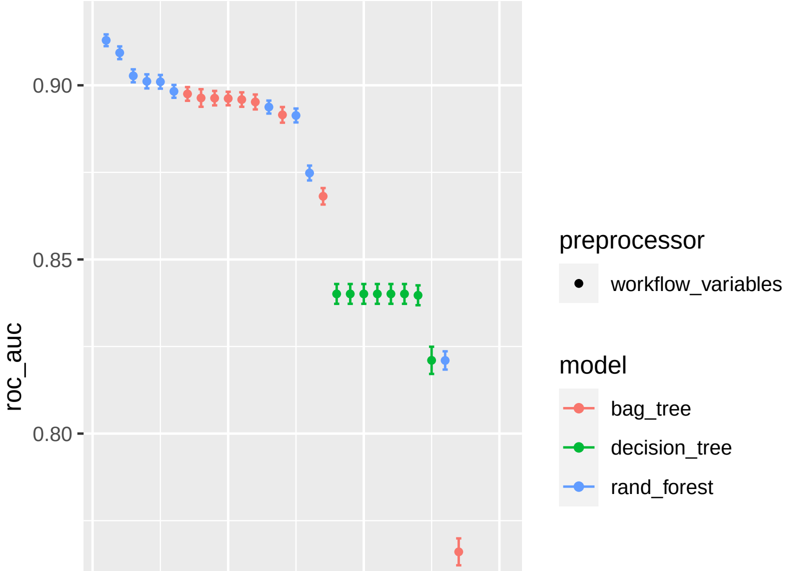
DONT RUN THIS CODE NOW

```
 # 3 parameter grid tuning
grid_ctrl <-
  control_grid(
    save_pred = TRUE,
    parallel_over = "everything",
    save_workflow = TRUE
  )

#will execute the same function across the workflows in the set
grid_results <-
  wkf %>%
  workflow_map(
    seed = 1503,
    resamples = apt_folds,
    grid = 10,
    control = grid_ctrl
  )

grid_results
```

```
#  3.1 print results: rank models and plot performance
# Rank models,
grid_results %>%
  rank_results( ) %>%  # every model
  filter(.metric == "roc_auc") %>%
  select(model, .config, rmse = mean, rank)
```

```
## # A tibble: 30 x 4
##    model       .config                rmse  rank
##    <chr>       <chr>                 <dbl> <int>
##  1 rand_forest Preprocessor1_Model06 0.913     1
##  2 rand_forest Preprocessor1_Model04 0.909     2
##  3 rand_forest Preprocessor1_Model01 0.903     3
##  4 rand_forest Preprocessor1_Model08 0.901     4
##  5 rand_forest Preprocessor1_Model03 0.901     5
##  6 rand_forest Preprocessor1_Model07 0.898     6
##  7 bag_tree    Preprocessor1_Model01 0.898     7
##  8 bag_tree    Preprocessor1_Model10 0.896     8
##  9 bag_tree    Preprocessor1_Model07 0.896     9
## 10 bag_tree    Preprocessor1_Model05 0.896    10
```

```r
# compare models
autoplot(
  grid_results,
  rank_metric = "roc_auc",  # <- how to order models
  metric = "roc_auc",       # <- which metric to visualize
)
```


roc_auc
0.90
0.85
0.80
preprocessor
● workflow_variables
model
bag_tree
decision_tree
rand_forest

```
# 4 Select the best model
# Select best RF parameters and fit the model on the training and test
rf_model <-
  grid_results %>%
  extract_workflow_set_result("simple_RF") %>% #ID in wkf obj
  select_best(metric = "roc_auc")

rf_test_results <-
  grid_results %>%
  extract_workflow("simple_RF") %>%
  finalize_workflow(rf_model) %>% #update tuning parameters in workflow
  last_fit(split = data_split_c) #fit with training and evaluate test
```

```
# Obtain predictions in the test
collect_metrics( rf_test_results )

# A tibble: 2 × 4
  .metric  .estimator .estimate .config
  <chr>    <chr>          <dbl> <chr>
1 accuracy binary         0.849 Preprocessor1_Model1
2 roc_auc  binary         0.920 Preprocessor1_Model1
```

- Specify a random forest for the apartment data regression problem
- Use the engine `randomForest`
- Tune the hyperparamenter `mtry` and `ntree` with a 10-k-fold CV with a grid for mtry (3, 5, 7,) and for ntree (100, 200, 500). Uss `expand.grid` for all the combinations.
- Select the best model
- Fit the best model and compare the predictive performance for the best model with a RF without tuning.

Yali Amit and Donald Geman. Shape quantization and recognition with randomized trees. *Neural computation*, 9(7):1545–1588, 1997.

Leo Breiman. Bagging predictors. *Machine learning*, 24(2):123–140, 1996.

Leo Breiman. Random forests. *Machine learning*, 45(1):5–32, 2001.

Leo Breiman et al. Heuristics of instability and stabilization in model selection. *The annals of statistics*, 24(6):2350–2383, 1996.

Tin Kam Ho. The random subspace method for constructing decision forests. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, 20(8): 832–844, 1998.

Robert E Schapire. The strength of weak learnability. *Machine learning*, 5(2): 197–227, 1990.