# DATA SOCIETY®

Advanced classification - day 2

"One should look for what is and not what he thinks should be."
-Albert Einstein.

# Module completion checklist

Objective	Complete
Optimize random forest model	
Predict and evaluate the optimized model	
Optimize gradient boosting model	
Predict and evaluate the optimized boosting model	

#### Directory settings

- In order to maximize the efficiency of your workflow, you should encode your directory structure into variables
- Let the main dir be the variable corresponding to your af-werx folder

```
# Set `main_dir` to the location of your `af-werx` folder (for Linux).
main_dir = "/home/[username]/Desktop/af-werx"

# Set `main_dir` to the location of your `af-werx` folder (for Mac).
main_dir = "/Users/[username]/Desktop/af-werx'

# Set `main_dir` to the location of your `af-werx` folder (for Windows).
main_dir = "C:\\Users\\[username]\\Desktop\\af-werx"

# Make `data_dir` from the `main_dir` and
# remainder of the path to data_directory.
data_dir = main_dir + "/data"
```

#### Loading packages

- Let's load the packages we will be using
- These packages are used for classification using decision trees, random forests, xgboost and other tools for classification best practices

```
import os
import pickle
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
from textwrap import wrap
from sklearn.model_selection import train_test_split
from sklearn import metrics
from sklearn import tree
from sklearn import tree
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import accuracy_score
from sklearn.ensemble import GradientBoostingClassifier
from matplotlib.legend_handler import HandlerLine2D
# New today
from sklearn.model_selection import RandomizedSearchCV
```

### Working directory

Set working directory to data dir

```
# Set working directory.
os.chdir(data_dir)

# Check working directory.
print(os.getcwd())

/home/[user-name]/Desktop/af-werx/data
```

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#### Random forest vs gradient boosting

#### **Goal for today**

- Optimize a random forest and gradient boosting model to predict high yield in Costa Rican dataset
- Compare models at the end of today and decide on a model champion

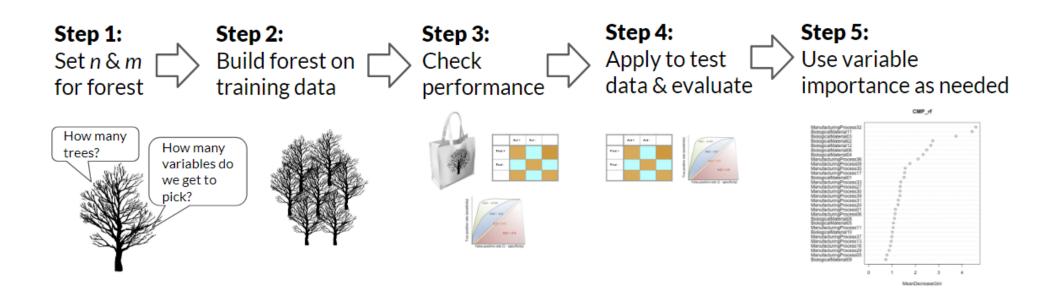
#### Recap: random forest

- We understand how one tree works
- Why not try a forest?

#### What is a random forest?

- Ensemble method used for classification and regression tasks
- Supervised learning algorithm which builds **multiple decision trees** and aggregates the result
- Uses a technique called Bootstrap Aggregation, commonly known as **Bagging**
- Limits overfitting and bias error

### Random forest methodology



#### Recap: why random forest?

- Reduction in overfitting
- Higher predictive accuracy
- Efficient with large datasets
- When should we use decision trees instead?
  - Intuitive and easily interpretable results
  - Less computationally expensive algorithm



#### Review data cleaning steps from last week

- Today, we will be loading the cleaned dataset we used last class
- To recap, the steps to get to this cleaned dataset were:
  - Remove household ID and individual ID
  - Remove variables with over 50% NAs.
  - Transformed target variable to binary
  - Remove highly correlated variables

#### Load the cleaned dataset

- Let's load the dataset from last week, costa no hc no highly correlated variables
- Save it as costa clean

#### Print info on data

Let's view the column names

```
costa clean.columns
```

```
Index(['rooms', 'tablet', 'males under 12', 'males over 12',
    'females under 12', 'females over 12', 'years of schooling',
    'wall block brick', 'wall socket', 'wall prefab cement', 'wall wood',
    'floor mos cer terr', 'floor wood', 'ceiling', 'electric public',
    'toilet sewer', 'cookenergy elec', 'trash truck', 'wall bad',
    'wall reg', 'roof bad', 'roof reg', 'floor bad', 'floor reg',
    'disabled ppl', 'male', 'under10', 'free', 'married', 'separated',
    'single', 'hh head', 'hh spouse', 'hh child', 'num 65plus',
    'dependency rate', 'male hh head educ', 'female hh head educ',
    'meaneduc', 'educ primary inc', 'educ primary', 'educ secondary inc',
    'educ secondary', 'educ undergrad', 'ppl per room', 'house owned full',
    'house owned paying', 'house rented', 'house other', 'computer',
    'television', 'num mobilephones', 'region central', 'region Chorotega',
    'region pacifico', 'region brunca', 'region antlantica',
    'region huetar', 'urban zone', 'age', 'Target'],
    dtype='object')
```

#### Split into training and test sets

```
# Select the predictors and target.
X = costa_clean.drop(['Target'], axis = 1)
y = np.array(costa_clean['Target'])

# Set the seed to 1.
np.random.seed(1)

# Split into training and test sets.
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.3)
```

#### Tuning random forest model

- We saw when we built our random forest that there are many parameters
- Let's load our original model from last week
- Now we can take a look at the parameters currently in use

```
forest = pickle.load(open("model_forest.sav","rb"))

forest.get_params()

{'bootstrap': True, 'class_weight': None, 'criterion': 'gini', 'max_depth': None, 'max_features': 'auto', 'max_leaf_nodes': None, 'min_impurity_decrease': 0.0, 'min_impurity_split': None, 'min_samples_leaf': 1, 'min_samples_split': 2, 'min_weight_fraction_leaf': 0.0, 'n_estimators': 100, 'n_jobs': None, 'oob_score': False, 'random_state': 1, 'verbose': 0, 'warm_start': False}
```

#### Tuning random forest model

- The best approach would be to narrow the range of values for each parameter
- We can use RandomizedSearchCV to optimize our hyperparameters to sample from during fitting
- GridSearchCV can be computationally expensive, especially when dealing with a large hyperparameter space
- We can search only a random subset of parameter values instead, using RandomSearchCV

#### RandomizedSearchCV

- It uses a randomized search on hyperparameters
- Unlike GridSearchCV, it samples a fixed number of parameter settings from specified probability distributions

#### sklearn.model\_selection.RandomizedSearchCV

class sklearn.model\_selection. RandomizedSearchCV (estimator, param\_distributions, n\_iter=10, scoring=None, fit\_params=None, n\_jobs=None, iid='warn', refit=True, cv='warn', verbose=0, pre\_dispatch='2\*n\_jobs', random\_state=None, error\_score='raise-deprecating', return\_train\_score='warn') { [source]

#### Parameter grid

Let's create a grid of parameter ranges

```
# Number of trees in random forest.
n estimators = [int(x) for x in np.linspace(start = 200, stop = 2000, num = 10)]
# Number of features to consider at every split.
max features = ['auto', 'sqrt']
# Maximum number of levels in tree.
max depth = [int(x) for x in np.linspace(10, 110, num = 11)]
max depth.append(None)
# Minimum number of samples required to split a node.
min samples split = [2, 5, 10]
# Minimum number of samples required at each leaf node.
min samples leaf = [1, 2, 4]
# Create the random grid.
random grid = {'n estimators': n estimators,
               'max features': max features,
               'max depth': max depth,
               'min samples split': min samples split,
               'min samples leaf': min samples leaf}
print(random grid)
```

#### Set up cross-validation function

Now we instantiate the model, using 3-fold cross-validation with 100 different combinations

```
rf_random.best_params_
```

```
{'n_estimators': 1000,
  'min_samples_split': 5,
  'min_samples_leaf': 2,
  'max_features': 'sqrt',
  'max_depth': 10}
```

#### Optimized random forest model

 Now we can use these optimized hyperparameters to implement the random forest again on X train

```
optimized_forest.fit(X_train, y_train)
```

# Knowledge Check 1



#### Exercise 1



# Module completion checklist

Objective	Complete
Optimize random forest model	<b>✓</b>
Predict and evaluate the optimized model	
Optimize gradient boosting model	
Predict and evaluate the optimized boosting model	

#### Predict using the best model parameters

Prediction class for each observation as a list.

```
optimized_forest_y_predict = optimized_forest.predict(X_test)
# Look at the first few predictions.
print(optimized_forest_y_predict[0:5, ])

[False False False False False]

optimized_forest_accuracy = metrics.accuracy_score(y_test, optimized_forest_y_predict)
print ("Accuracy on test data (best model): ", optimized_forest_accuracy)
Accuracy on test data (best model): 0.8535564853556485
```

#### Optimized random forest: save final accuracy

- Let's save our random forest score in our model\_final dataset
- We first have to load our model\_final dataframe from last week

```
model_final_optimized =
pickle.load(open("model_final_forest_gbm.sav","rb"))
```

#### Optimized random forest: save final accuracy

```
metrics values
                                           model
   accuracy 0.6046
                                           knn 5
   accuracy 0.6188
                                knn GridSearchCV
2
3
4
   accuracy 0.6287
                                          knn 29
                                        logistic
   accuracy 0.6356
   accuracy 0.7845
                         logistic whole dataset
   accuracy 0.7859
                                  Togistic tuned
                             tree simple subset
   accuracy 0.6611
   accuracy 0.9407
                             tree all variables
                     tree all variables optimized
   accuracy 0.7183
   accuracy 0.9338
                                  random forest
   accuracy 0.8644
                                        boosting
   accuracy 0.8536
                           optimized forest
```

# Knowledge Check 2



#### Exercise 2



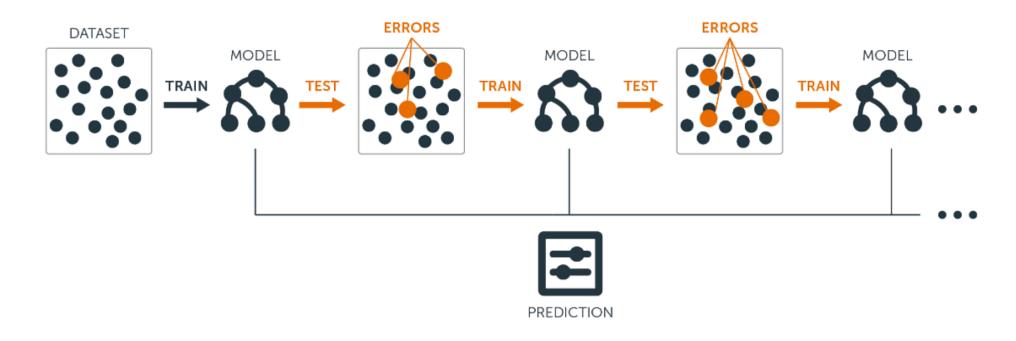
# Module completion checklist

Objective	Complete
Optimize random forest model	
Predict and evaluate the optimized model	<b>✓</b>
Optimize gradient boosting model	
Predict and evaluate the optimized boosting model	

#### Recap: boosting intuition

- In simple linear regression, you can clearly see the residuals, which are the multiple points around the linear model
- Let's think of these residuals, but apply the concept to decision trees
- When **gradient boosting** uses decision trees, it follows these three steps:
  - it sees the **errors from a decision tree** on the dataset
  - it identifies the pattern of the errors and builds a new decision tree on them
  - it repetitively leverages these patterns in residuals to strengthen the overall model

#### Gradient boosted trees



#### Source

#### Recap: boosting process

- The process of gradient boosting is math heavy and complex
- However, for now, it can be simplified to three steps that we just discussed:
- 1. Fit a decision tree model to the data
- 2. Fit a decision tree model to the residuals
- 3. Create a new model

- Gradient boosting can be used with classification or regression
- The generalization of the multiple weak learners occurs by the optimization of a differentiable loss function
- The **loss function** will change based on the model's target variable:
  - Regression: gradient descent used to minimize MSE
  - Binary classification: logistic function

### Ways to optimize gradient boosting

- We saw when we built our boosting model that there are many parameters
- All the values of our original boosting model are set to the GradientBoostingClassifier defaults within sklearn
- We are now going to optimize the model focusing on the four parameters we called out
  - max depth = None
  - min samples split = 2
  - min samples leaf = 1
  - max\_features = None

#### Define an optimal number function

- Before we optimize individual parameters, let's build a function that will help us store the parameters we will be using in our optimized\_gbm
- The inputs are:
  - values: list of values for given parameter that we iterate through
  - test results: predictions on test set for each parameter that we iterate over
- The output is:
  - best\_value: the actual parameter value that performs best and that we will use in our final optimized boosting model

```
# Define function that will determine the optimal number for each parameter.
def optimal_parameter(values, test_results):
   best_test_value = max(test_results)
   best_test_index = test_results.index(best_test_value)
   best_value = values[best_test_index]
   return(best_value)
```

#### Optimize: learning rate

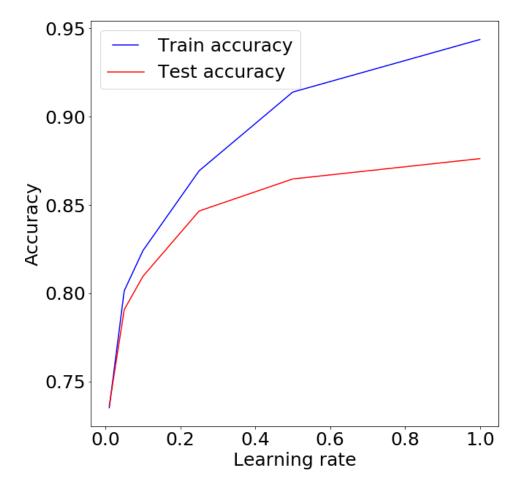
```
# Learning Rate
learning_rates = [1, 0.5, 0.25, 0.1, 0.05, 0.01]
train_results = []

for eta in learning_rates:
    model = GradientBoostingClassifier(learning_rate=eta)
    model.fit(X_train, y_train)
    train_pred = model.predict(X_train)
    acc_train = accuracy_score(y_train, train_pred)
    train_results.append(acc_train)
    y_pred = model.predict(X_test)
    acc_test = accuracy_score(y_test, y_pred)
    test_results.append(acc_test)
```

```
optimal_learning_rate = optimal_parameter(learning_rates, test_results)
```

#### Plot: learning rate

```
from matplotlib.legend_handler import
HandlerLine2D
line1, = plt.plot(learning_rates,
train_results,'b', label= "Train accuracy")
line2, = plt.plot(learning_rates, test_results,
'r', label= "Test accuracy")
plt.legend(handler_map={line1:
HandlerLine2D(numpoints=2)})
plt.ylabel("Accuracy")
plt.xlabel("Learning_rate")
plt.show()
```



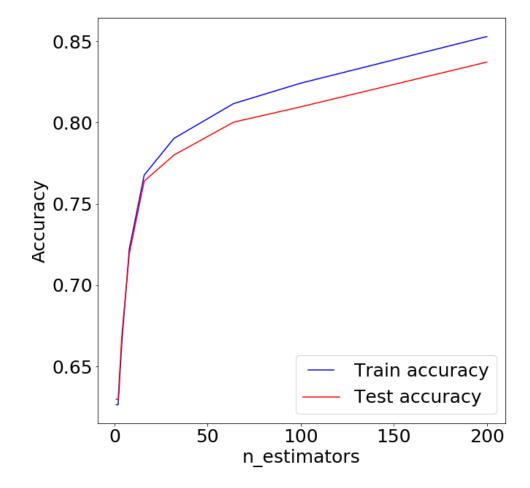
#### Optimize: n estimators

```
n_estimators = [1, 2, 4, 8, 16, 32, 64, 100, 200]
train_results = []
test_results = []
for estimator in n_estimators:
    model = GradientBoostingClassifier(n_estimators=estimator)
    model.fit(X_train, y_train)
    train_pred = model.predict(X_train)
    acc_train = accuracy_score(y_train, train_pred)
    train_results.append(acc_train)
    y_pred = model.predict(X_test)
    acc_test = accuracy_score(y_test, y_pred)
    test_results.append(acc_test)
```

```
optimal_n_estimators = optimal_parameter(n_estimators, test_results)
```

#### Plot: n estimators

```
from matplotlib.legend_handler import
HandlerLine2D
line1, = plt.plot(n_estimators, train_results,
'b', label= "Train accuracy")
line2, = plt.plot(n_estimators, test_results,
'r', label= "Test accuracy")
plt.legend(handler_map={line1:
HandlerLine2D(numpoints=2)})
plt.ylabel('Accuracy')
plt.xlabel('n_estimators')
plt.show()
```



## Optimize: max depth

- max depth indicates how deep the tree can be
- The deeper the tree, the more splits it has, which captures more information about the data
- But remember, there is a fine line between a well fit model and an overfit model
- In our original model,  $max\_depth = None now$ , we are going to fit a decision tree with depths ranging from 1 to 32 and plot the training and test accuracy

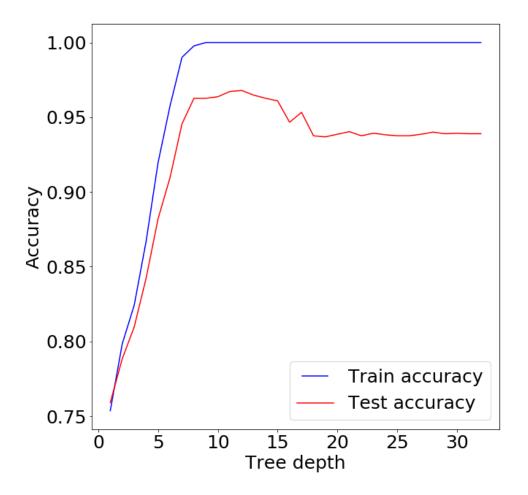
```
# Max depth:
max_depths = np.linspace(1, 32, 32, endpoint=True)
train_results = []
test_results = []
for max_depth in max_depths:
    model = GradientBoostingClassifier(max_depth=max_depth)
    model.fit(X_train, y_train)
    train_pred = model.predict(X_train)
    acc_train = accuracy_score(y_train, train_pred)
    train_results.append(acc_train)
    y_pred = model.predict(X_test)
    acc_test = accuracy_score(y_test, y_pred)
    test_results.append(acc_test)
```

```
# Store optimal max_depth.
optimal_max_depth = optimal_parameter(max_depths, test_results)
```

## Plot: max depth

- Let's plot the max depth train\_results and test results
- This will allow us to see when the model starts overfitting on train as well as when the optimal test results are achieved
- What observations can you make?

```
# Plot max depth over 1-32.
line1, = plt.plot(max_depths, train_results,
'b', label= "Train accuracy")
line2, = plt.plot(max_depths, test_results, 'r',
label= "Test accuracy")
plt.legend(handler_map={line1:
HandlerLine2D(numpoints=2)})
plt.ylabel('Accuracy')
plt.xlabel('Tree depth')
plt.show()
```



## Optimize: min samples split

- min samples split: minimum number of samples required to split an internal node
  - This can vary between considering at least one sample at each node to considering all samples at each node
  - When we **increase this parameter, the tree becomes more constrained** as it has to consider more samples at each node
  - We will vary the parameter from 10% to 100% of the samples

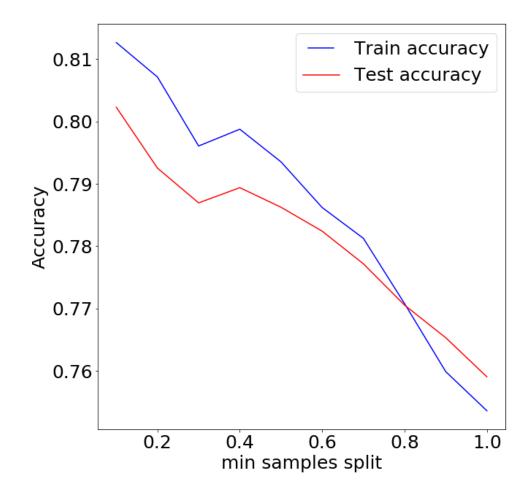
```
min_samples_splits = np.linspace(0.1, 1.0, 10, endpoint = True)
train_results = []
test_results = []
for min_samples_split in min_samples_splits:
    model = GradientBoostingClassifier(min_samples_split = min_samples_split)
    model.fit(X_train, y_train)
    train_pred = model.predict(X_train)
    acc_train = accuracy_score(y_train, train_pred)
    train_results.append(acc_train)
    y_pred = model.predict(X_test)
    acc_test = accuracy_score(y_test, y_pred)
    test_results.append(acc_test)
```

```
# Store optimal min_samples_split.
optimal_min_samples_split = optimal_parameter(min_samples_splits, test_results)
```

## Plot: min samples split

- Let's plot the min samples split train results and test results
  - What observations can you make?

```
line1, = plt.plot(min_samples_splits,
train_results, 'b', label = "Train accuracy")
line2, = plt.plot(min_samples_splits,
test_results, 'r', label = "Test accuracy")
plt.legend(handler_map = {line1:
HandlerLine2D(numpoints = 2)})
plt.ylabel('Accuracy')
plt.xlabel('min samples split')
plt.show()
```



## Optimize: min samples leaf

- min\_samples\_leaf is the minimum number of samples required to be at a lead node
- This parameter is similar to min\_samples\_split except that this parameter describes the minimum number of samples at the leafs the base of the tree

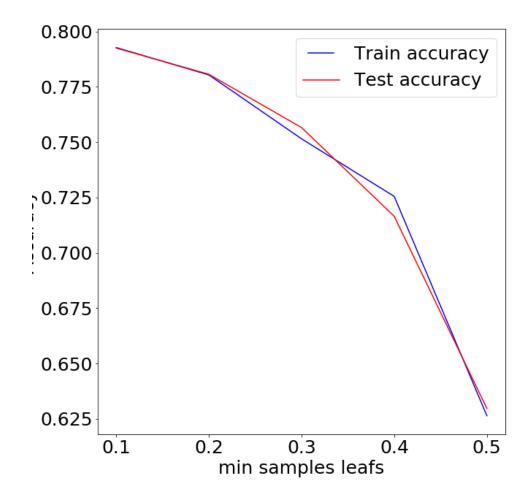
```
# Min_samples_leaf:
min_samples_leafs = np.linspace(0.1, 0.5, 5, endpoint = True)
train_results = []
test_results = []
for min_samples_leaf in min_samples_leafs:
    model = GradientBoostingClassifier(min_samples_leaf = min_samples_leaf)
    model.fit(X_train, y_train)
    train_pred = model.predict(X_train)
    acc_train = accuracy_score(y_train, train_pred)
    train_results.append(acc_train)
    y_pred = model.predict(X_test)
    acc_test = accuracy_score(y_test, y_pred)
    test_results.append(acc_test)
```

```
optimal_min_samples_leafs = optimal_parameter(min_samples_leafs, test_results)
```

## Plot: min samples leaf

- Let's plot the min samples leaf train results and test results
- What observations can you make?

```
line1, = plt.plot(min_samples_leafs,
train_results, 'b', label = "Train accuracy")
line2, = plt.plot(min_samples_leafs,
test_results, 'r', label = "Test accuracy")
plt.legend(handler_map = {line1:
HandlerLine2D(numpoints = 2)})
plt.ylabel('Accuracy')
plt.xlabel('min_samples_leafs')
plt.show()
```



## Optimize: max features

- max\_features represents the number of features to consider when looking for the best split
- This parameter is set to None as its default value, so the tree will always look through all features
- This could sometimes cause overfitting and/or is computationally expensive when working with many variables

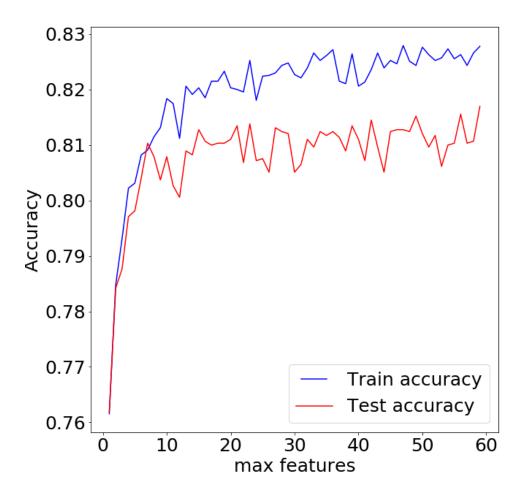
```
# Max_features:
max_features = list(range(1, X.shape[1]))
train_results = []
test_results = []
for max_feature in max_features:
    model = GradientBoostingClassifier(max_features = max_feature)
    model.fit(X_train, y_train)
    train_pred = model.predict(X_train)
    acc_train = accuracy_score(y_train, train_pred)
# Add acc_score_to_previous_train_results.
train_results.append(acc_train)
y_pred = model.predict(X_test)
acc_test = accuracy_score(y_test, y_pred)
# Add acc_score_to_previous_test_results.
test_results.append(acc_test)
```

```
optimal_max_features = optimal_parameter(max_features, test_results)
```

#### Plot: max features

- Let's plot the max features train results and test results
  - What observations can you make?

```
line1, = plt.plot(max_features, train_results,
'b', label = "Train accuracy")
line2, = plt.plot(max_features, test_results,
'r', label = "Test accuracy")
plt.legend(handler_map = {line1:
HandlerLine2D(numpoints = 2)})
plt.ylabel('Accuracy')
plt.xlabel('max features')
plt.show()
```



## Optimized model

- Now that we have now walked through four parameters that will help us optimize our gradient boosting model
- Let's look at what each of the optimal parameters are:

```
print("The optimal learning rate is:",
  optimal_learning_rate)

The optimal learning rate is: 1

print("The optimal number of estimators is:",
  optimal_n_estimators)
The optimal number of estimators is: 200
```

```
print ("The optimal max depth is:",
optimal max depth)
The optimal max depth is: 3.0
print ("The optimal min samples split is:",
optimal min samples split)
The optimal min samples split is: 0.1
print ("The optimal min samples leaf is:",
optimal min samples leafs)
The optimal min samples leaf is: 0.1
print ("The optimal max features is:",
optimal max features)
The optimal max features is: 59
```

# Knowledge Check 3



## Exercise 3



## Module completion checklist

Objective	Complete
Optimize random forest model	<b>✓</b>
Predict and evaluate the optimized model	<b>/</b>
Optimize gradient boosting model	<b>/</b>
Predict and evaluate the optimized boosting model	

## Build optimized model

Now, we will run the optimized model on our x train

```
GradientBoostingClassifier(criterion='friedman_mse', init=None, learning_rate=1, loss='deviance', max_depth=3.0, max_features=59, max_leaf_nodes=None, min_impurity_decrease=0.0, min_impurity_split=None, min_samples_leaf=0.1, min_samples_split=0.1, min_weight_fraction_leaf=0.0, n_estimators=200, n_iter_no_change=None, presort='auto', random_state=None, subsample=1.0, tol=0.0001, validation_fraction=0.1, verbose=0, warm_start=False)
```

```
gbm_optimized_fit = gbm_optimized.fit(X_train, y_train)
```

## Predict with optimized model

- Finally, let's predict on x test and calculate our accuracy score
- How is our optimized model doing?
- What other metrics can you also look at?

```
# Predict on X_test.
y_predict_gbm_optimized = gbm_optimized.predict(X_test)

# Accuracy score.
acc_score_gbm_optimized = accuracy_score(y_test, y_predict_gbm_optimized)
print(acc_score_gbm_optimized)
```

0.8563458856345886

## Add accuracy score to the final scores

- So we have it, let's add this score to the dataframe model final that we created earlier
- Let's append the score to model final optimized

```
metrics values
                                         model
accuracy 0.6046
                                         knn 5
accuracy 0.6188
                              knn GridSearchCV
accuracy 0.6287
                                        knn 29
accuracy 0.6356
                                      logistic
                        logistic whole dataset
accuracy 0.7845
accuracy 0.7859
                                Togistic tuned
accuracy 0.6611
                            tree simple subset
                            tree all variables
accuracy 0.9407
                  tree all variables optimized
accuracy 0.7183
accuracy 0.9338
                                 random forest
accuracy 0.8644
                                      boosting
accuracy 0.8536
                             optimized forest
accuracy 0.8563
                                 gbm optimized
```

Now that we have built all our models and have our final accuracy, let's discuss our results

## Discuss model champion

- When we look for the best model, we do not just want to take the model with the highest accuracy score
- Remember to consider:
  - bias in models
  - optimized vs. biased models
- We now want to open the class up for discussion about which model you would choose, and why

#### Final scores

```
print(model_final_optimized)
```

```
metrics values
                                      model
accuracy 0.6046
                                      knn 5
                            knn GridSearchCV
accuracy 0.6188
accuracy 0.6287
                                     knn 29
                                   logistic
accuracy 0.6356
                  logistic whole dataset
accuracy 0.7845
accuracy 0.7859
                              Togistic tuned
                        tree simple subset
accuracy 0.6611
accuracy 0.9407
                        tree all variables
                tree all variables optimized
accuracy 0.7183
                         random forest
accuracy 0.9338
accuracy 0.8644
                                   boosting
                          optimized forest
accuracy 0.8536
accuracy 0.8563
                              gbm optimized
```

```
pickle.dump(model_final_optimized, open("model_final_optimized_ensemble.sav", "wb"))
```

# Knowledge Check 4



### Exercise 4



## Module completion checklist

Objective	Complete
Optimize random forest model	<b>✓</b>
Predict and evaluate the optimized model	<b>/</b>
Optimize gradient boosting model	<b>/</b>
Predict and evaluate the optimized boosting model	<b>/</b>

### Workshop: next steps!

- Workshops are to be completed in the afternoon either with a dataset for a capstone project or with another dataset of your choosing
- Make sure to annotate and comment your code
- This is an exploratory exercise to get you comfortable with the content we discussed today
  - Step 1: Load data, clean data to get ready for exploratory data analysis
  - Step 2: Look for patterns by using visualizations and also unsupervised learning
  - Step 3: Using any insights gained from steps 1 and 2, move forward with building a base data table for modeling
  - Step 4: Determine your target variable, this will be the variable of interest, what you want to predict
  - Step 5: Build classification models using class materials as guidance, save accuracy scores like we did with out model final dataframes
  - Step 6: Determine a model champion

# This completes our module **Congratulations!**