

cases/data points that are hard to predict correctly.

- Next, we will talk about **Gradient Boosting**. You learned about gradient descent in the earlier module. The same principle applies here as well, where the newly added trees are trained to **reduce the errors (loss function)** of earlier models. So, overall, in gradient boosting, we are optimizing the performance of the boosted model by bringing down the loss one small step at a time.
- **XGBoost** is an extended version of **gradient boosting**, where it uses more accurate approximations to tune the model and find the best fit.

## Why is XGBoost so good?

1. **Parallel Computing:** when you run xgboost, by default, it would use all the cores of your laptop/machine enabling its capacity to do parallel computation
2. **Regularization:** The biggest advantage of xgboost is that it uses regularization and controls the overfitting and simplicity of the model which gives it better performance.
3. **Enabled Cross-Validation:** XGBoost is enabled with internal Cross Validation function
4. **Missing Values:** XGBoost is designed to handle missing values internally. The missing values are treated in such a manner that if there exists any trend in missing values, it is captured by the model.
5. **Flexibility:** XGBoost is not just limited to regression, classification, and ranking problems, it supports user-defined objective functions as well. Furthermore, it supports user-defined evaluation metrics as well.

Because of parallel processing (speed) and model performance, we can say that XGBoost is gradient boosting on steroids.

The screenshot shows a digital assessment interface. At the top, it says "Question 2/2" and has a "Mandatory" button. Below that, there are two rows of question status indicators. The first row for "Question 1" shows a list icon, the text "Question 1", a red "X" icon, the word "Incorrect", and a right-pointing arrow. The second row for "Question 2" shows a list icon, the text "Question 2", a green checkmark icon, the word "Correct", and a right-pointing arrow. A blue checkmark icon is also visible in the top right corner of the interface.

Now, that you have gone through the basic intuition behind XGBoost, let's study how to implement it practically.

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PREVIOUS  
Gradient Boosting Algorithm



NEXT  
XGBoost Lab

# Introduction

Until now, you have learned the original boosting algorithm, AdaBoost.

In this session, we will learn another popular boosting algorithm - **Gradient Boosting** and a modification of Gradient Boosting called **XGBoost** which is widely used in the industry. We will also briefly discuss some of the more advanced algorithms recently introduced.

Towards the end, we will go through the implementation of the different algorithms on a Kaggle Dataset in Python.

## In this session

Let's look at the broad flow of this session.





## Prerequisites

Understanding how gradient descent works is a prerequisite for this session. You would have gone through the topic in the Linear Regression module.

## Guidelines for in-module questions

The in-video and in-content questions for this module are not graded.

## People you will hear from in this session

### Subject Matter Expert:

Prof G Srinivasaraghavan

Professor, IIIT- B

The International Institute of Information Technology, Bangalore, commonly known as IIIT Bangalore, is a premier national graduate school in India. Founded in 1999, it offers Integrated M.Tech., M.Tech., M.S. (Research) and PhD programs in the field of Information Technology.

Anjali Rajvanshi

Sr. Subject Matter Expert, upGrad

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Q&A

Snehansu Sekhar Sahu

Sr. Research Engineer in ML & AI at American Express

Snehanshu has more than 6 years of experience and has worked with companies like Qualcomm Inc, Infoedge solutions & American Express. He is currently part of the ML & AI Research Group @ AmEx.



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# Understanding Gradient Boosting - I





# Understanding Gradient Boosting - I

Gradient Boosting like AdaBoost trains many models in a gradual, additive, and sequential manner. But the major difference between the two is how they identify & handle the shortcomings of weak learners. In AdaBoost, we provide more say or weight to those data points which are misclassified/ wrongly predicted earlier. Gradient boosting performs the same by using gradients in the loss function.

In the next video, Anjali will explain the fundamentals of the Gradient boosting machine and how does it work.





The loss function is a measure indicating how good the model is able to fit the underlying data. This varies from one problem statement to another problem statement and thus would depend on what we are trying to optimize. In the case of a regression problem, the loss function would be the error between true and predicted target values. For classification problems, the loss function would be a measure of how good our predictive model is at classifying each sample point that we have in our dataset.

Let's now understand GBM with the help of a numerical example for a regression problem.





To summarize here are the broader points on how does a GBM learn:

- Build the first weak learner using a sample from the training data; we will consider a decision tree as the weak learner or the base model. It may not necessarily be a stump, can grow a bigger tree but will still be weak i.e. still not be fully grown.
- Then the predictions are made on the training data using the decision tree just built.
- The gradient, in our case the residuals are computed and these **residuals are the new response or target values for the next weak learner.**
- A new weak learner is built with the residuals as the target values and a sample of observations from the original training data.
- Add the predictions obtained from the current weak learner to the predictions obtained from all the previous weak learners. The predictions obtained at each step are multiplied by the learning rate so that no single model makes a huge contribution to the ensemble thereby avoiding overfitting. Essentially, with the addition of each weak learner, the model takes a very small step in the right direction.
- The next weak learner fits on the residuals obtained till now and these steps are repeated, either for a prespecified number of weak learners or if the model starts overfitting i.e. it starts to capture the niche patterns of the training data.
- GBM makes the final prediction by simply adding up the predictions from all the weak learners (multiplied by the learning rate).

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# Understanding Gradient Boosting - I

Gradient Boosting like AdaBoost trains many models in a gradual, additive, and sequential manner. But the major difference between the two is how they identify & handle the shortcomings of weak learners. In AdaBoost, we provide more say or weight to those data points which are misclassified/ wrongly predicted earlier. Gradient boosting performs the same by using gradients in the loss function.

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# Understanding Gradient Boosting - II

In this session, we will go through the algorithm of gradient boosting in a regression setting. With the intuition learned from the previous videos, let us see how this translates to the algorithm behind the model.





At any iteration  $t$ , we repeat the following steps in the Gradient Boosting scheme of things:

1. Initialize a crude initial function  $F_0$  as  $\operatorname{argmin} \sum_{t=1}^T \mathbf{L}(\mathbf{y}_i, \hat{\mathbf{y}})$

- This will be the average value which will form our first predicton.

1. For  $m = 1$  to  $M$  (where  $M$  is the number of trees)

1. Calculate the pseudo-residuals  $r_{im} = -\frac{(\partial \mathbf{L}(\mathbf{y}_i, \mathbf{F}(\mathbf{x}_i)))}{\partial \mathbf{F}(\mathbf{x}_i)}$ , where  $\mathbf{F}(\mathbf{x}_i) = F_{m-1}(\mathbf{x}_i)$

, the pseudo residuals are the negative gradients for all data points

2. Fit a base learner  $h_m(x)$  to the pseudo-residuals, i.e train it using the training set

$\sum_{i=1}^n (x_i, r_{im})$ . Here the pseudo residuals are used as the response variable.

3. Compute the step magnitude multiplier  $\gamma_m$  (in case of tree models, compute a  $\gamma_m$  different for every leaf/prediction). In other words, introducing step multiplier results in a small step in the right direction.

$$\gamma_m = \operatorname{argmin} \sum_{i=1}^n L(y_i, (F_{m-1} + \gamma * h_m(x_i)))$$

4. Compute the next model  $F_m = F_{m-1}(x_i) + \gamma_m * h_m(x_i)$

2. The final model is  $F_M(x)$

We see here that the gradient boosting algorithm essentially starts off with a crude model that gives a certain output  $y_{avg}$ , which is the mean of all the target values.

The next function  $F_1$  is developed such that it models the **residuals**,  $y_i - y_{avg}$ .

The point to note here is that the new model  $F_1$ , builds a regression model on the feature vectors of their **residual**. Hence the target variable for  $F_1$  is the residual,  $y_i - y_i^0$  and not the actual target variable  $y_i$ . We can write the residual  $y_i - y_i^0$  as  $y_i - F_0(x_i)$ .

&lt; &gt;

**Question 1/3**

Mandatory



## Gradient Boosting Steps

In continuation to the above video, after we fit the model  $F_1$  on the residuals  $y_i - F_0(x_i)$ , the prediction we get for  $x_i$  is  $F_1(x_i)$ . What do you think is the residual now?

  $y_i - F_0(x_i) - F_1(x_i)$  **Correct**

## Feedback:

The target variable for  $F_1$  was  $y_i - F_0(x_i)$ . Hence, the residual will be target variable - predicted value which is  $y_i - F_0(x_i) - F_1(x_i)$ .

  $y_i - F_1(x_i)$ **Your answer is Correct.****Attempt 1 of 1****Continue**

Now that you have got a brief understanding of how gradient boosting works, let's study what the *gradient* in gradient boosting is.

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## Question 2/3

Mandatory



## Gradient Boosting Steps

Now, like we created a new function  $F_1$  and trained it on  $y_i - F_0(x_i)$ , we create a new function  $F_2$  as the next model to be trained in the Gradient Boosting Algorithm. What do you think  $F_2$  will train on?

 $y_i$  $y_i - F_1(x_i)$  $y_i - F_0(x_i) - F_1(x_i)$ 

✓ Correct

**Feedback:**

In every step/iteration of Gradient Boosting, we fit the new model on the residual of the corresponding step. So here  $F_2$  will fit on the residual  $y_i - F_0(x_i) - F_1(x_i)$ .



Your answer is Correct.

Attempt 2 of 2

Continue

Now that you have got a brief understanding of how gradient boosting works, let's study what the *gradient* in gradient boosting is.



## Question 3/3

Mandatory



## General Expression for Residual

Let us generalize the above expression for a model  $F_t$ . What is the general expression of the target variable the model  $F_t$  trains on? Assume,  $y$  is the initial target variable.

  $y - [F_0 + F_{t-1}]$   $y - [F_0 + F_1 + F_2 + \dots + F_{t-2} + F_{t-1}]$ 

✓ Correct

## Feedback:

$F_1$  trains on  $y - F_0$ ,  $F_2$  trains on  $y - F_0 - F_1 = y - [F_0 + F_1]$ , and so on. In general,  $F_t$  trains on the residuals generated by the model  $F_{t-1}$  which is  $y - [F_0 + F_1 + F_2 + \dots + F_{t-2} + F_{t-1}]$ .



Your answer is Correct.

Attempt 1 of 1

Continue

Now that you have got a brief understanding of how gradient boosting works, let's study what the *gradient* in gradient boosting is.

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# Gradient in Gradient Boosting

We got an intuition of how the gradient boosting process helps in reducing the error with each iteration. To summarise, the gradient boosting algorithm has two steps at each iteration:

1. Find the residual and fit a new model on the residual
2. Add the new model to the older model and continue the next iteration

Let's now see how this can be seen as a **gradient descent problem**.

## Comprehension - Gradient Descent

You have learned that in the gradient descent algorithm, a function  $G(x)$  decreases fastest around a point  $a$  if one goes along the negative gradient of  $G(x)$ . It follows the iterative process:

$$a_{n+1} = a_n - \lambda \frac{dG(x)}{dx}$$

Now if the function is  $G(x, y)$ , we have the following formulation:

$$x_{n+1} = x_n - \lambda \frac{\partial G(x, y)}{\partial x}$$

Keeping these in mind answer the following questions:



### Question 1/2

Mandatory



#### Gradient Descent of univariate function

Let  $g(x) = x^3 + e^{-x}$ .

Which direction should we move to minimize  $g(x)$  at a point with the x-coordinate  $x$ ?

  $3x^2 + e^{-x}$   $3x^2 - e^{-x}$   $e^{-x} - 3x^2$ 

Correct



Feedback:

We should be moving in the direction of negative gradient which is  $e^{-x} - 3x^2$



Your answer is Correct.

Attempt 2 of 2

Continue



We see that the negative gradient of the square loss function gives the residue. So the strategy of closing in on the residues at each step can be seen as taking a **step towards the negative gradient of the loss function**. We can observe here that gradient descent helps in generalising the boosting process.

Please **note** that this explanation and the aforementioned process of closing in on the residues is only valid for square error loss function.

## Additional Reading

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Gradient Boosting  
Algorithm



Keeping these in mind answer the following questions:



## Question 2/2

Mandatory



### Gradient Descent of bivariate function

Let,  $g(x) = x^3 + y^2$ .

Which direction should we move in to minimize this function at a point  $(x,y)$ ?

Note that the answer will be a vector in which  $i$  represents the  $x$ -direction and  $j$  represents the  $y$ -direction.

$x^3i + y^2j$

$-(3x^2i + 2yj)$

✓ Correct

! Feedback:

We have  $-\frac{\partial}{\partial x}g(x, y) = -3x^2$  and  $-\frac{\partial}{\partial y}g(x, y) = -2y$ . Hence, we move in the direction  $-(3x^2i + 2yj)$

$xi + yj$



Your answer is Correct.

Attempt 1 of 2

Continue

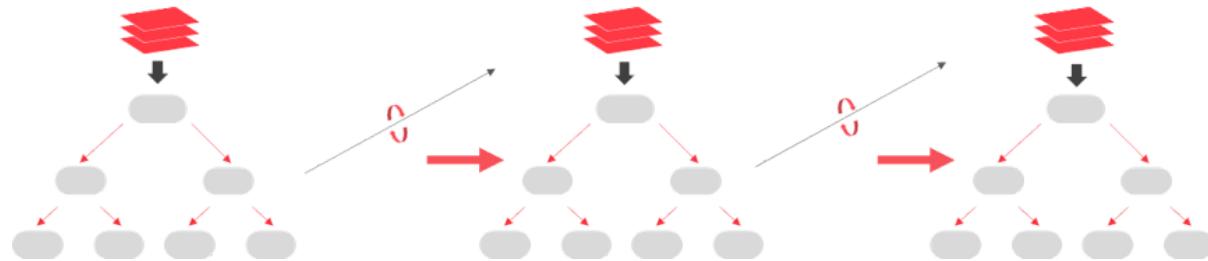
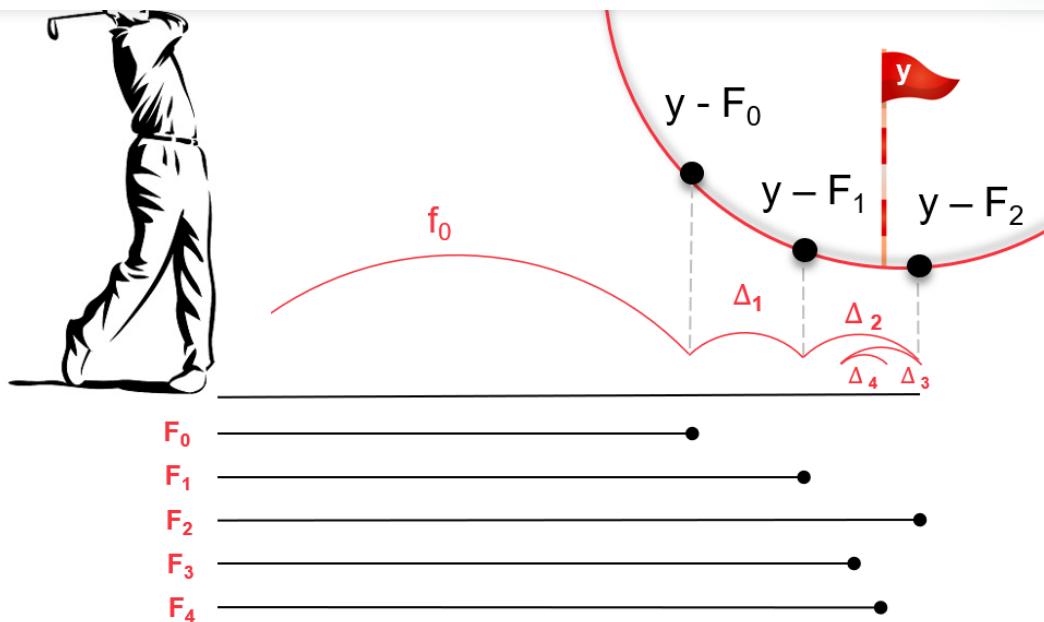
# Gradient Boosting Algorithm

The **negative gradients** at an iteration  $t$  act as a **target variable** to fit a model  $h_m$  and for a regression setting with a square loss function, this target variable was the residue.

To explain this in just words, at each iteration we add an incremental model, which fits on the negative gradients of the loss function evaluated at current target values. This incremental model can be a linear regression model or a decision tree or any other model.

We stop when we see that the gradients are very close to zero. For a regression setting, this means that when the residuals are very close to zero, we stop iterating. Here,  $\gamma_m$ , known as the **step multiplier**, is typically between 0 and 1.

In other words, introducing step multiplier results in a small step in the right direction.  $\gamma$  corresponds to the hyperparameter  $\alpha$  in terms of the utility (both determine by what amount an update should be made), but here  $\gamma$  is trainable while  $\alpha$  is a hyperparameter.



Here at each iteration, a new model(weak learner) is added and with each new addition, we can observe a reduction in the pseudo residuals which is an indication that we are moving in the right direction of the target values.

Refer to the original documentation for both Regression & Classification,

You can try out GBM for classification using the notebook below



[Attrition prediction using GBM](#)



[Download](#)



You can try out GBM for regression using the notebook below

**Sales prediction using GBM**

Download

The dataset used for the Sales prediction can be downloaded [here](#)

## Additional Reading

For practical implementation please go through this [blog](#).

Visit this [kernel](#) to see how each parameter is can be tuned for model improvement.

To check how we can do gradient boosting from scratch, you can check this [article](#).

To play with different hyperparameters in Gradient Boosting, visit this [website](#).

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[Understanding XGBoost](#)

The issue of keeping one's employees happy and satisfied is a perennial and age-old challenge. If an employee you have invested so much time and money leaves for "greener pastures", then this would mean that you would have to spend even more time and money to hire somebody else.

This project is based on a hypothetical dataset downloaded from IBM HR Analytics Employee Attrition & Performance. It has 1,470 data points (rows) and 35 features (columns) describing each employee's background and characteristics; and labelled (supervised learning) with whether they are still in the company or whether they have gone to work somewhere else.

**Problem statement** To understand and determine how these factors relate to workforce attrition.

Dataset: <https://www.kaggle.com/patelprashant/employee-attrition>  
[\(https://www.kaggle.com/patelprashant/employee-attrition\)](https://www.kaggle.com/patelprashant/employee-attrition)

In [2]:

```
#Importing the Libraries
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
%matplotlib inline
import plotly.offline as py
import plotly.graph_objs as go
from sklearn.model_selection import train_test_split
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import (accuracy_score, log_loss, confusion_matrix)
#Suppressing warnings
import warnings
warnings.filterwarnings('ignore')
```

In [4]:

```
#Importing the Dataset
df = pd.read_csv('WA_Fn-UseC_-HR-Employee-Attrition.csv')
```

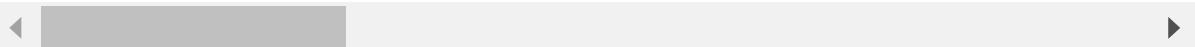
In [5]:

```
df.head(3)
```

Out[5]:

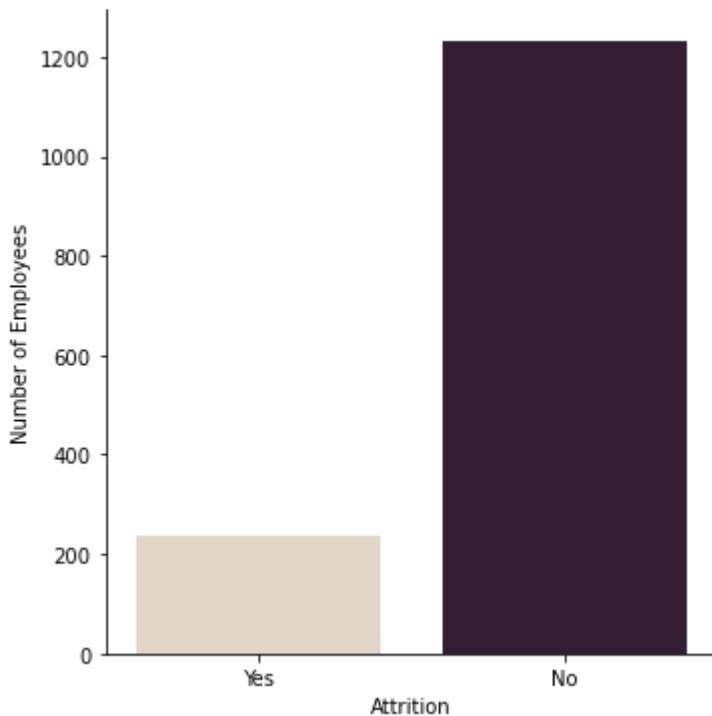
	Age	Attrition	BusinessTravel	DailyRate	Department	DistanceFromHome	Education	Edu
0	41	Yes	Travel_Rarely	1102	Sales	1	2	L
1	49	No	Travel_Frequently	279	Research & Development	8	1	L
2	37	Yes	Travel_Rarely	1373	Research & Development	2	2	

3 rows × 35 columns



In [6]:

```
#Checking the number of 'Yes' and 'No' in 'Attrition'
ax = sns.catplot(x="Attrition", kind="count", palette="ch:.25", data=df);
ax.set(xlabel = 'Attrition', ylabel = 'Number of Employees')
plt.show()
```



any missing values in the dataframe.

In [7]:

```
#Identifying columns with missing information
missing_col = df.columns[df.isnull().any()].values
print('The missing columns in the dataset are: ',missing_col)
```

The missing columns in the dataset are: []

## Step 2 - Feature Engineering

The numeric and categorical fields need to be treated separately and the target field needs to be separated from the training dataset. The following few steps separate the numeric and categorical fields and drops the target field 'Attrition' from the feature set.

In [8]:

```
#Extracting the Numeric and Categorical features
df_num = pd.DataFrame(data = df.select_dtypes(include = ['int64']))
df_cat = pd.DataFrame(data = df.select_dtypes(include = ['object']))
print("Shape of Numeric: ",df_num.shape)
print("Shape of Categorical: ",df_cat.shape)
```

Shape of Numeric: (1470, 26)  
 Shape of Categorical: (1470, 9)

### 2.1 Encoding Categorical Fields

The categorical fields have been encoded using the `get_dummies()` function of Pandas.

In [9]:

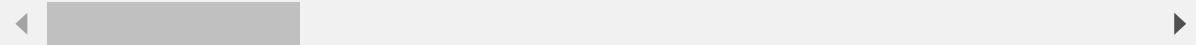
```
#Dropping 'Attrition' from df_cat before encoding
df_cat = df_cat.drop(['Attrition'], axis=1)

#Encoding using Pandas' get_dummies
df_cat_encoded = pd.get_dummies(df_cat)
df_cat_encoded.head(5)
```

Out[9]:

	BusinessTravel_Non-Travel	BusinessTravel_Travel_Frequently	BusinessTravel_Travel_Rarely	Departr
0	0	0	0	1
1	0	1	0	0
2	0	0	1	1
3	0	1	0	0
4	0	0	0	1

5 rows × 29 columns



### 2.2 Scaling Numeric Fields

The numeric fields have been scaled next for best results. `StandardScaler()` has been used for the same. Post scaling of the numeric features, they are merged with the categorical ones.

In [10]:

```
#Using StandardScaler to scale the numeric features
standard_scaler = StandardScaler()
df_num_scaled = standard_scaler.fit_transform(df_num)
df_num_scaled = pd.DataFrame(data = df_num_scaled, columns = df_num.columns, index = df_num.index)
print("Shape of Numeric After Scaling: ",df_num_scaled.shape)
print("Shape of categorical after Encoding: ",df_cat_encoded.shape)
```

Shape of Numeric After Scaling: (1470, 26)  
 Shape of categorical after Encoding: (1470, 29)

In [11]:

```
#Combining the Categorical and Numeric features
df_transformed_final = pd.concat([df_num_scaled,df_cat_encoded], axis = 1)
print("Shape of final dataframe: ",df_transformed_final.shape)
```

Shape of final dataframe: (1470, 55)

In [12]:

```
#Extracting the target variable - 'Attrition'
target = df['Attrition']

#Mapping 'Yes' to 1 and 'No' to 0
map = {'Yes':1, 'No':0}
target = target.apply(lambda x: map[x])

print("Shape of target: ",target.shape)

#Copying into commonly used fields for simplicity
X = df_transformed_final #Features
y = target #Target
```

Shape of target: (1470,)

## 2.3 Train and Test Split

The data is next split into training and test dataset using the train\_test\_split functionality of sklearn.

In [13]:

```
#Splitting into Train and Test dataset in 90-10 ratio
X_train, X_test, y_train, y_test = train_test_split(X,y,train_size = 0.8, random_state = 0,
print("Shape of X Train: ",X_train.shape)
print("Shape of X Test: ",X_test.shape)
print("Shape of y Train: ",y_train.shape)
print("Shape of y Test: ",y_test.shape)
```

Shape of X Train: (1176, 55)  
 Shape of X Test: (294, 55)  
 Shape of y Train: (1176,)  
 Shape of y Test: (294,)

## Step 3 - Model Fitting

In [16]:

```
#Using Gradient Boosting to predict 'Attrition' and create the Trees to identify important
gbm = GradientBoostingClassifier(n_estimators = 200, max_features = 0.7, learning_rate = 0.

#Fitting Model
gbm.fit(X_train, y_train)

#pred
y_pred = gbm.predict(X_test)
```

In [17]:

```
print('Accuracy of the model is: ',accuracy_score(y_test, y_pred))
```

Accuracy of the model is: 0.8469387755102041

In [18]:

```
#Confusion Matrix
cm = confusion_matrix(y_test, y_pred)
print('The confusion Matrix : \n',cm)
```

The confusion Matrix :

```
[[241  6]
 [ 39  8]]
```

## Step 4 - Visualisation and Identification of Important Features

Here, I have used the 'feature\_importances\_' array of the Gradient Boosting Model to ascertain the most important features for the prediction of 'Attrition'.

In [20]:

```
# Scatter plot
trace = go.Scatter(
    y = gbm.feature_importances_,
    x = df_transformed_final.columns.values,
    mode='markers',
    marker=dict(
        sizemode = 'diameter',
        sizeref = 1,
        size = 12,
        color = gbm.feature_importances_,
        colorscale='Portland',
        showscale=True
    ),
    text = df_transformed_final.columns.values
)
data = [trace]

layout= go.Layout(
    autosize= True,
    title= 'Model Feature Importance',
    hovermode= 'closest',
    xaxis= dict(
        ticklen= 5,
        showgrid=False,
        zeroline=False,
        showline=False
    ),
    yaxis=dict(
        title= 'Feature Importance',
        showgrid=False,
        zeroline=False,
        ticklen= 5,
        gridwidth= 2
    ),
    showlegend= False
)
fig = go.Figure(data=data, layout=layout)
py.iplot(fig,filename='scatter')
```



Online property companies offer valuations of houses using machine learning techniques. The dataset consisted of historic data of houses sold between May 2014 to May 2015. We will predict the sales of houses in King County with an accuracy of at least 75-80% and understand which factors are responsible for higher property value - \$650K and above."

**Problem statement** The aim of this report is to predict the house sales in King County, Washington State, USA using different models (Adaboost & GBM)

Dataset: <https://www.kaggle.com/shivachandel/kc-house-data> (<https://www.kaggle.com/shivachandel/kc-house-data>)

## STEP 1: IMPORTING LIBRARIES

In [30]:

```
import numpy as np
import pandas as pd
import xgboost
import math
import seaborn as sns
import matplotlib
import matplotlib.pyplot as plt
from __future__ import division
from scipy.stats import pearsonr
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split
# from sklearn.cross_validation import ShuffleSplit
from sklearn.metrics import explained_variance_score
from time import time
from sklearn.metrics import r2_score
import os
from sklearn.model_selection import train_test_split

# from sklearn import cross_validation, tree, Linear_model
```

In [9]:

```
data = pd.read_csv('kc_house_data.csv')
```

In [10]:

```
# Copying data to another dataframe df_train for our convinience so that original dataframe
df_train=data.copy()
df_train.rename(columns ={'price': 'SalePrice'}, inplace =True)
```

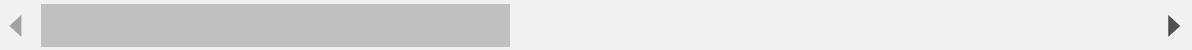
In [11]:

```
# Now lets see the first five rows of the data
data.head()
```

Out[11]:

	<b>id</b>	<b>date</b>	<b>price</b>	<b>bedrooms</b>	<b>bathrooms</b>	<b>sqft_living</b>	<b>sqft_lot</b>	<b>floors</b>
<b>0</b>	7129300520	20141013T000000	221900.0	3	1.00	1180	5650	1.0
<b>1</b>	6414100192	20141209T000000	538000.0	3	2.25	2570	7242	2.0
<b>2</b>	5631500400	20150225T000000	180000.0	2	1.00	770	10000	1.0
<b>3</b>	2487200875	20141209T000000	604000.0	4	3.00	1960	5000	1.0
<b>4</b>	1954400510	20150218T000000	510000.0	3	2.00	1680	8080	1.0

5 rows × 21 columns



## STEP 2: DATA CLEANING AND PREPROCESSING

In [12]:

```
print(len(data))
# Check the number of features in the data set
print(len(data.columns))
# Check the data types of each column
print(data.dtypes)
```

```
21613
21
id          int64
date        object
price       float64
bedrooms    int64
bathrooms   float64
sqft_living int64
sqft_lot    int64
floors      float64
waterfront  int64
view        int64
condition   int64
grade       int64
sqft_above  int64
sqft_basement int64
yr_built    int64
yr_renovated int64
zipcode    int64
lat         float64
long        float64
sqft_living15 int64
sqft_lot15   int64
dtype: object
```

In [15]:

```
# Check any number of columns with NaN or missing values
print(data.isnull().any().sum(), ' / ', len(data.columns))
```

0 / 21

In [14]:

```
# Check any number of data points with NaN
print(data.isnull().any(axis=1).sum(), ' / ', len(data))
```

0 / 21613

### STEP 3 : FINDING CORRELATION

In [16]:

```
# As id and date columns are not important to predict price so we are discarding it for finding correlations
features = data.iloc[:,3:].columns.tolist()
target = data.iloc[:,2].name
```

In [17]:

```
# Finding Correlation of price woth other variables to see how many variables are strongly correlated
correlations = {}
for f in features:
    data_temp = data[[f,target]]
    x1 = data_temp[f].values
    x2 = data_temp[target].values
    key = f + ' vs ' + target
    correlations[key] = pearsonr(x1,x2)[0]
```

In [18]:

```
# Printing all the correlated features value with respect to price which is target variable
data_correlations = pd.DataFrame(correlations, index=['Value']).T
data_correlations.loc[data_correlations['Value'].abs().sort_values(ascending=False).index]
```

Out[18]:

	Value
<b>sqft_living vs price</b>	0.702035
<b>grade vs price</b>	0.667434
<b>sqft_above vs price</b>	0.605567
<b>sqft_living15 vs price</b>	0.585379
<b>bathrooms vs price</b>	0.525138
<b>view vs price</b>	0.397293
<b>sqft_basement vs price</b>	0.323816
<b>bedrooms vs price</b>	0.308350
<b>lat vs price</b>	0.307003
<b>waterfront vs price</b>	0.266369
<b>floors vs price</b>	0.256794
<b>yr_renovated vs price</b>	0.126434
<b>sqft_lot vs price</b>	0.089661
<b>sqft_lot15 vs price</b>	0.082447
<b>yr_builtin vs price</b>	0.054012
<b>zipcode vs price</b>	-0.053203
<b>condition vs price</b>	0.036362
<b>long vs price</b>	0.021626

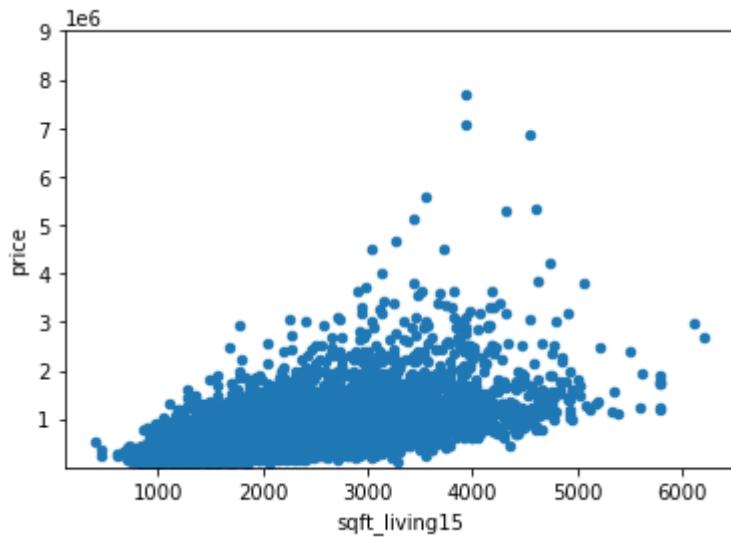
As zipcode is negatively correlated with sales price , so we can remove it for sales price prediction.

\*STEP 4 : EDA or DATA VISUALIZATION \*

Let's explore the data

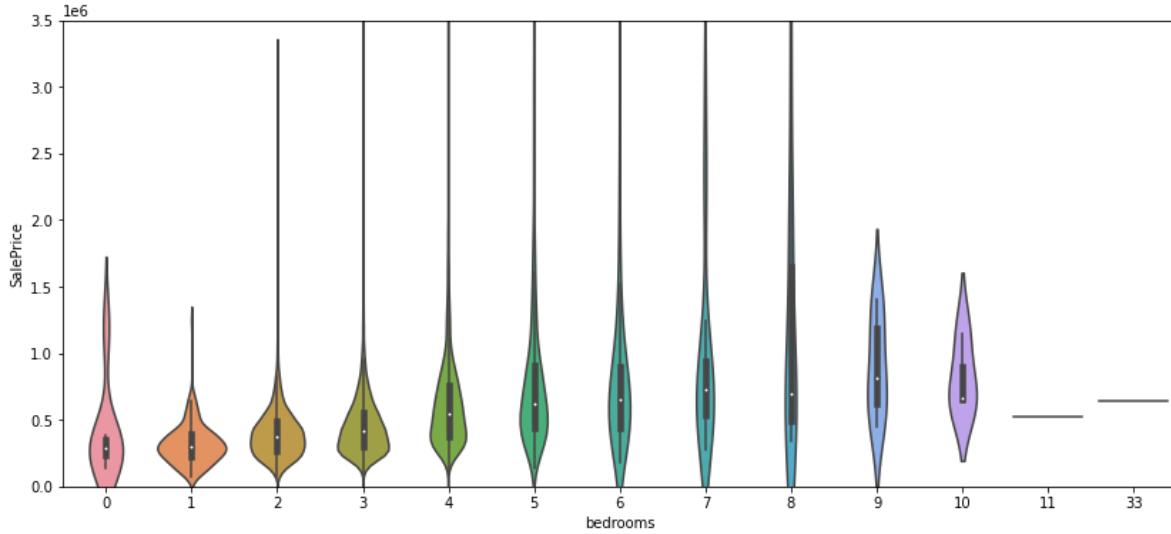
In [19]:

```
var = 'sqft_living15'  
data = pd.concat([data['price'], data[var]], axis=1)  
data.plot.scatter(x=var, y='price', ylim=(3,9000000));
```



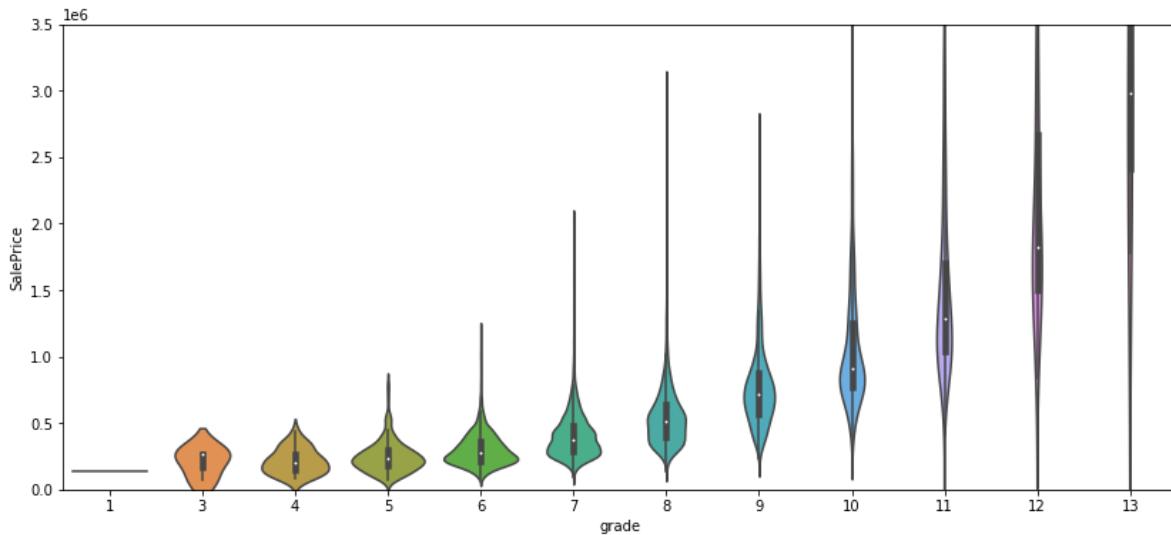
In [20]:

```
var = 'bedrooms'
data = pd.concat([df_train['SalePrice'], df_train[var]], axis=1)
f, ax = plt.subplots(figsize=(14, 6))
fig = sns.violinplot(x=var, y="SalePrice", data=data)
fig.axis(ymin=0, ymax=3500000);
```



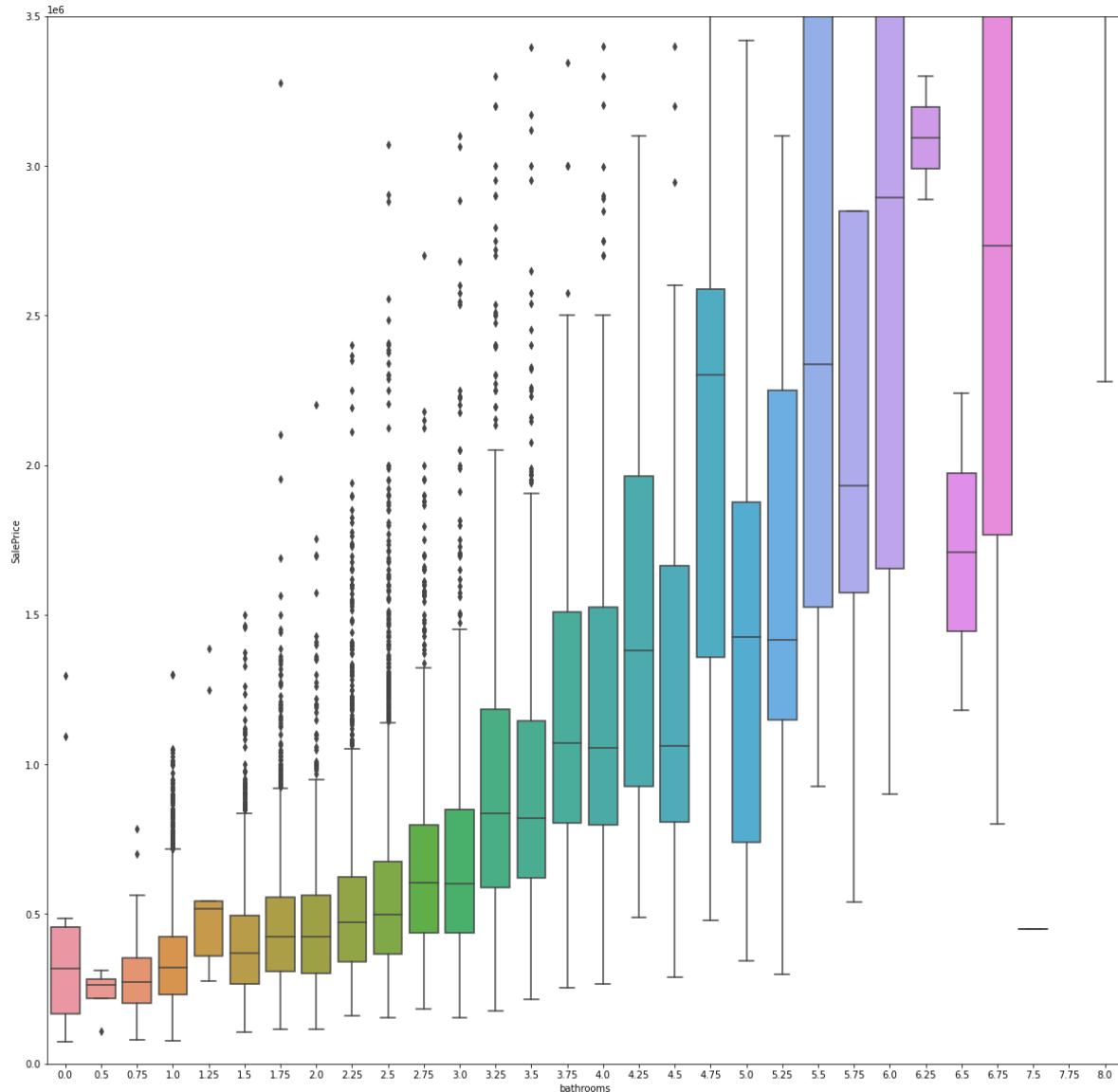
In [21]:

```
var = 'grade'
data = pd.concat([df_train['SalePrice'], df_train[var]], axis=1)
f, ax = plt.subplots(figsize=(14, 6))
fig = sns.violinplot(x=var, y="SalePrice", data=data)
fig.axis(ymin=0, ymax=3500000);
```



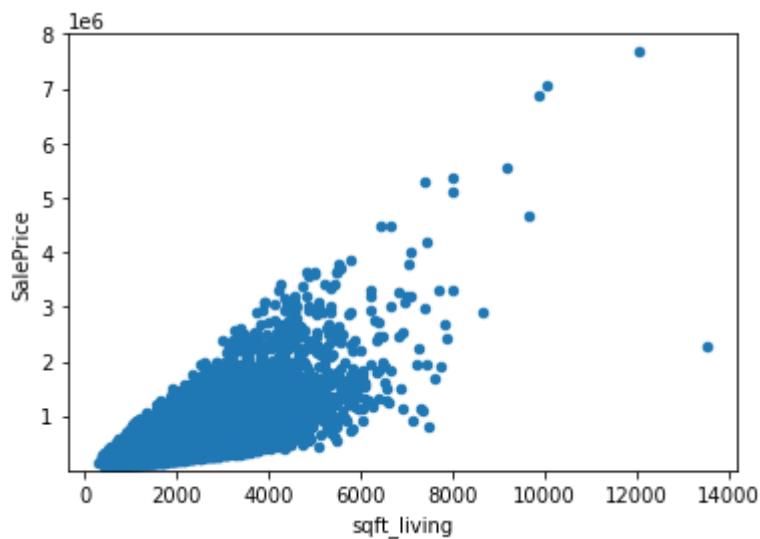
In [22]:

```
var = 'bathrooms'
data = pd.concat([df_train['SalePrice'], df_train[var]], axis=1)
f, ax = plt.subplots(figsize=(20, 20))
fig = sns.boxplot(x=var, y="SalePrice", data=data)
fig.axis(ymin=0, ymax=3500000);
```



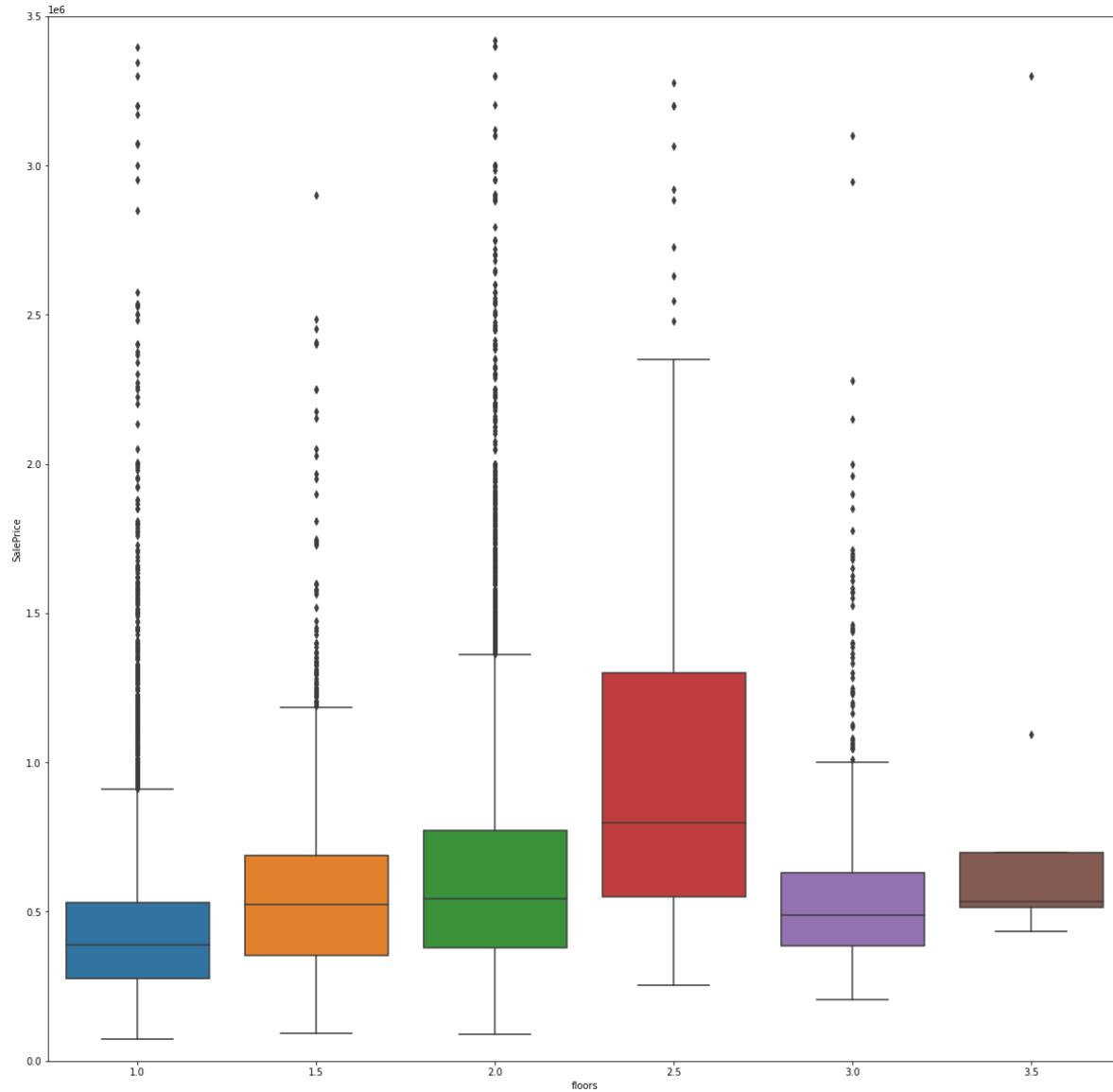
In [23]:

```
var = 'sqft_living'  
data = pd.concat([df_train['SalePrice'], df_train[var]], axis=1)  
data.plot.scatter(x=var, y='SalePrice', ylim=(3,8000000));
```



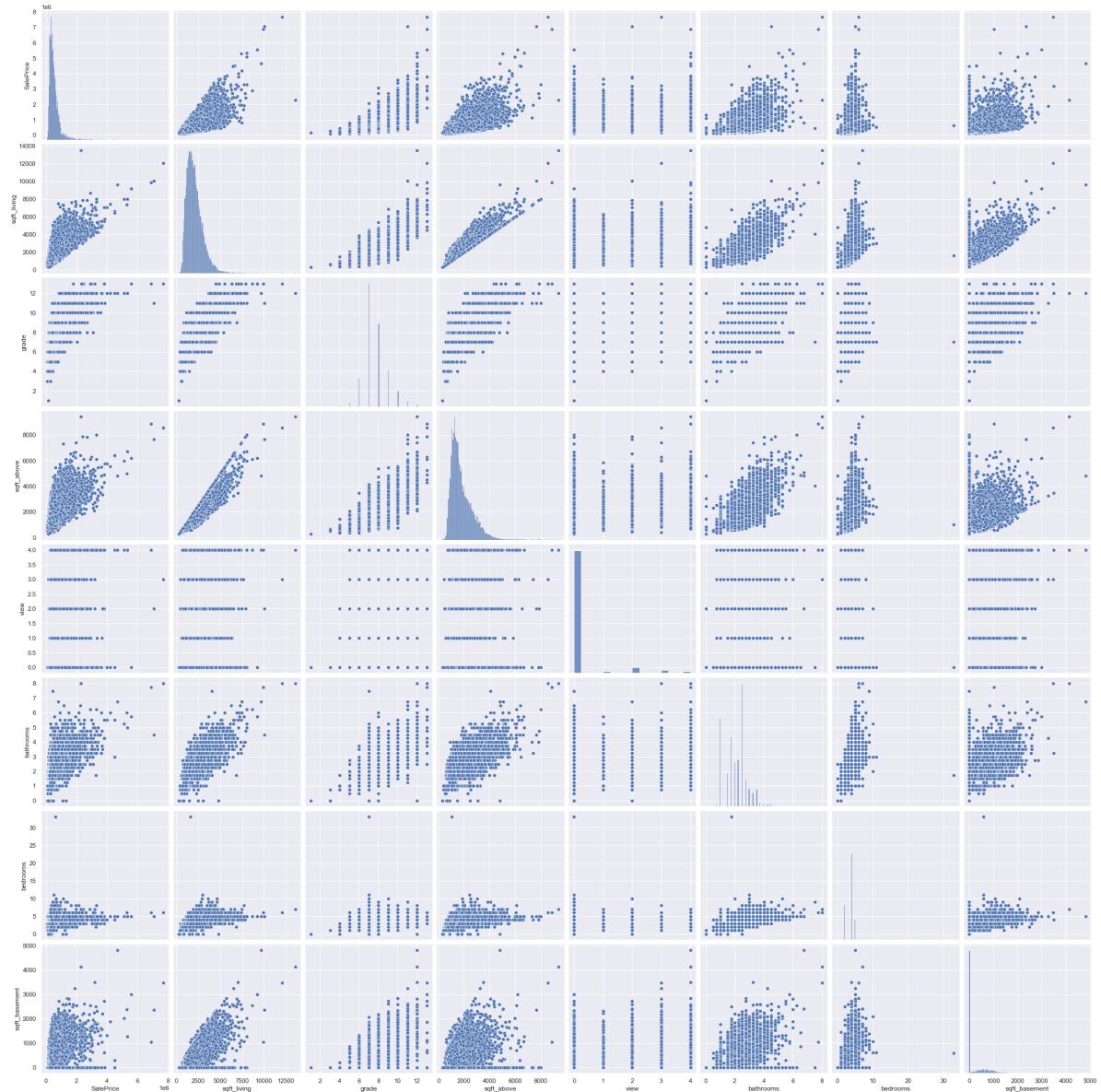
In [24]:

```
var = 'floors'
data = pd.concat([df_train['SalePrice'], df_train[var]], axis=1)
f, ax = plt.subplots(figsize=(20, 20))
fig = sns.boxplot(x=var, y="SalePrice", data=data)
fig.axis(ymin=0, ymax=3500000);
```



In [25]:

```
#Pairplots to visualize strong correlation
sns.set()
cols = ['SalePrice', 'sqft_living', 'grade', 'sqft_above', 'view', 'bathrooms', 'bedrooms', 'sqft_basement']
sns.pairplot(df_train[cols], height = 3.5)
plt.show();
```



In [27]:

```
filtered_data = df_train[['sqft_living', 'grade', 'sqft_above', 'sqft_living15', 'bathrooms',
```

In [28]:

```
X = filtered_data.values
y = df_train.SalePrice.values
```

**STEP 5 : SPLITTING DATA INTO TRAINING AND TESTING SET**

In [31]:

```
X_train, X_test, y_train, y_test = train_test_split(X, y ,test_size=0.2)
```

**STEP 6: APPLYING MACHINE LEARNING MODEL****Adaboost**

In [32]:

```
from sklearn.ensemble import AdaBoostRegressor
ada=AdaBoostRegressor(n_estimators=50, learning_rate=0.2,loss='exponential').fit(X_train, y
pred=ada.predict(X_test)
adab=ada.score(X_test,y_test)
predict = ada.predict(X_test)
exp_ada = explained_variance_score(predict,y_test)
```

**GBM**

In [33]:

```
from sklearn.ensemble import GradientBoostingRegressor
gbm=GradientBoostingRegressor(n_estimators=400, max_depth=5, loss='ls',min_samples_split=2,
gradient=gbm.score(X_test,y_test)

pred = gbm.predict(X_test)
exp_est = explained_variance_score(pred,y_test)
```

In [34]:

```
# Comparing Models on the basis of Model's Accuracy Score and Explained Variance Score of different models
models_cross = pd.DataFrame({
    'Model': ['Gradient Boosting','AdaBoost'],
    'Score': [gradient,adab],
    'Variance Score': [exp_est,exp_ada]})

models_cross.sort_values(by='Score', ascending=False)
```

Out[34]:

	Model	Score	Variance Score
0	Gradient Boosting	0.888402	0.879083
1	AdaBoost	0.655424	0.518544





# Understanding XGBoost

**Extreme Gradient Boosting (XGBoost)** is similar to the gradient boosting framework but more efficient and advanced implementation of the Gradient Boosting algorithm. It was first developed by Taiqi Chen and became famous in solving the Higgs Boson problem. Due to its robust accuracy, it has been widely used in machine learning competitions as well.

In the next video, with this understanding, let's see how does XGBoost works



Models are added sequentially to correct the errors made by previous models. This sequence of weak learners will produce a strong learner.



It is an extension of Gradient Boosted Machines, with parallel processing, better optimisation & regularization.



Newly added trees are trained to reduce the errors (loss function) of earlier models. The performance of model is optimised by bringing down the loss function.

- **AdaBoost** is an iterative way of adding weak learners to form the final model. For this, each model is trained to correct the errors made by the previous one. This sequential model does this by adding more weight to cases with incorrect predictions. By this approach, the ensemble model will correct itself while learning by focusing on cases/data points that are hard to predict correctly.
- Next, we will talk about **Gradient Boosting**. You learned about gradient descent in the earlier module. The same principle applies here as well, where the newly added trees are trained to **reduce the errors (loss function)** of earlier models. So, overall, in gradient boosting, we are optimizing the performance of the boosted model by bringing down the loss one small step at a time.
- **XGBoost** is an extended version of **gradient boosting**, where it uses more accurate approximations to tune the model and find the best fit.



2. **Regularization:** The biggest advantage of xgboost is that it uses regularization and controls the overfitting and simplicity of the model which gives it better performance.

3. **Enabled Cross-Validation:** XGBoost is enabled with internal Cross Validation function

4. **Missing Values:** XGBoost is designed to handle missing values internally. The missing values are treated in such a manner that if there exists any trend in missing values, it is captured by the model.

5. **Flexibility:** XGBoost is not just limited to regression, classification, and ranking problems, it supports user-defined objective functions as well. Furthermore, it supports user-defined evaluation metrics as well.

Because of parallel processing (speed) and model performance, we can say that XGBoost is gradient boosting on steroids.

< > Question 1/2 Mandatory ✓

### Features of XGBoost

Which of the following is/are a mandatory data pre-processing step(s) for XGBOOST?

Impute Missing Values ✗ Incorrect



Navigate

Q&amp;A

 Remove highly correlated predictors.

Incorrect

Feedback:

Decision trees are by nature immune to multicollinearity. Since boosted trees use individual decision trees, they also are unaffected by multicollinearity.

 One-hot encoding or dummy variable creation of categorical predictors

Correct

You missed this!

Feedback:

Yes converting categorical data to numeric format is required

 Normalization and scaling

Incorrect

Feedback:

For the decision tree algorithm, normalization is not necessary in the training model procedure.

Your answer is Wrong.

Attempt 2 of 2

Continue

Now, that you have gone through the basic intuition behind XGBoost, let's study how to implement it practically.

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2. **Regularization:** The biggest advantage of xgboost is that it uses regularization and controls the overfitting and simplicity of the model which gives it better performance.

3. **Enabled Cross-Validation:** XGBoost is enabled with internal Cross Validation function

4. **Missing Values:** XGBoost is designed to handle missing values internally. The missing values are treated in such a manner that if there exists any trend in missing values, it is captured by the model.

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Because of parallel processing (speed) and model performance, we can say that XGBoost is gradient boosting on steroids.



## Question 2/2

Mandatory



### True/False

The major difference between the Gradient Boosting and the XGBoost is that XGBoost incorporates the regularisation parameter in its objective function to control over-fitting

 True

✓ Correct



# XGBoost Lab

The objective of this segment is to learn how to implement the XGBoost algorithm in python.

But before that, let's look at some of the hyperparameters used in XGBoost.

## Hyperparameters - Learning Rate, Number of Trees and Subsampling

$\lambda_t$ , the **learning rate**, is also known as **shrinkage**. It can be used to regularize the gradient tree boosting algorithm.  $\lambda_t$  typically varies from 0 to 1. Smaller values of  $\lambda_t$  lead to a larger value of a number of trees T (called *n\_estimators* in the Python package XGBoost). This is because, with a slower learning rate, you need a larger number of trees to reach the minima. This, in turn, leads to longer training time.

On the other hand, if  $\lambda_t$  is large, we may reach the same point with a lesser number of trees (*n\_estimators*), but there's the risk that we might actually miss the minima altogether (i.e. cross over it) because of the long stride we are taking at each iteration.

Some other ways of regularization are explicitly specifying the **number of trees T** and doing **subsampling**. Note that you shouldn't tune both  $\lambda_t$  and number of trees T together since a high  $\lambda_t$  implies a low value of T and vice-versa.



therefore look similar. This is not a big problem in boosting since each tree is anyway built on the residual and gets a significantly different objective function than the previous one.

$\gamma$ , **Gamma** is a parameter used for controlling the pruning of the tree. A node is split only when the resulting split gives a positive reduction in the loss function. Gamma specifies the minimum loss reduction required to make a split and makes the algorithm conservative. The values can vary depending on the loss function and should be tuned.

Apart from the above-mentioned hyperparameters, there are other parameters of decision trees like the depth of the tree, the minimum number of samples required for split etc.

**NOTE:** The mathematical understanding behind XGboost is provided in the optional section.

For a detailed understanding, please attend the live session on Saturday.



## Question 1/2

Mandatory



### Hyperparameter Tuning in XGBoost

The hyperparameters  $\lambda_t$  (learning rate) and  $T$  (number of trees):



...and the number of trees.

Feedback:

The faster the learning rate, the faster you move towards the minima, thus requiring a lower number of trees.

- Are dependent on each other - the faster the learning rate, the higher the number of trees

Incorrect

Feedback:

The faster the learning rate, the faster you move towards the minima, thus requiring a lower number of trees.

Your answer is Wrong.

Attempt 1 of 1

Continue

With all this understanding let's move to the next video where Snehanshu will give you a walkthrough on how to do classification with XGBoost.





Now, that you have gone through classification, let's dive into the regression problem.

Snehanshu will now explain how we approach regression problem with XGBoost through a code walkthrough.



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XGBoost - regression



Download

Download and implement the code in the following notebook to get an understanding of both XGBoost classification & regression.

! [Report an error](#)



PREVIOUS

Understanding XGBoost Kaggle Practice Exercise

NEXT





therefore look similar. This is not a big problem in boosting since each tree is anyway built on the residual and gets a significantly different objective function than the previous one.

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Apart from the above-mentioned hyperparameters, there are other parameters of decision trees like the depth of the tree, the minimum number of samples required for split etc.

**NOTE:** The mathematical understanding behind XGboost is provided in the optional section.

For a detailed understanding, please attend the live session on Saturday.



## Question 2/2

Mandatory



### XGBoost Regularization

What will happen if we increase the regularisation parameter  $\lambda_t$ ?



Navigate

Q&amp;A

- 
- The number of trees will increase



Your answer is Correct.

Attempt 1 of 1

Continue

With all this understanding let's move to the next video where Snehanshu will give you a walkthrough on how to do classification with XGBoost.



In [1]:

```
import numpy as np
import pandas as pd
from sklearn.datasets import load_breast_cancer

pd.set_option('display.max_columns', None)
pd.set_option('display.max_rows', None)
```

In [2]:

## # Read the Dataset

```
data = load_breast_cancer()  
data
```

Out[2]:

ractal dimension ("coastline approximation" - 1)\n\n The mean, standa  
rd error, and "worst" or largest (mean of the three\n worst/largest v  
alues) of these features were computed for each image,\n resulting in  
30 features. For instance, field 0 is Mean Radius, field\n 10 is Rad  
ius SE, field 20 is Worst Radius.\n - class:\n - WDB  
C-Malignant\n - WDBC-Benign\n :Summary Statistics:\n\n  
===== Min Max\n =====\n rad  
ius (mean): 6.981 28.11\n texture (mean):  
9.71 39.28\n perimeter (mean): 43.79 188.5\n ar  
ea (mean): 143.5 2501.0\n smoothness (mean):  
0.053 0.163\n compactness (mean): 0.019 0.345\n co  
ncavity (mean): 0.0 0.427\n concave points (mean):  
0.0 0.201\n symmetry (mean): 0.106 0.304\n fr  
actal dimension (mean): 0.05 0.097\n radius (standard erro  
r): 0.112 2.873\n texture (standard error): 0.3  
6 4.885\n perimeter (standard error): 0.757 21.98\n area  
(standard error): 6.802 542.2\n smoothness (standard erro  
r): 0.002 0.031\n compactness (standard error): 0.002  
0.135\n concavity (standard error): 0.0 0.396\n concave p  
oints (standard error): 0.0 0.053\n symmetry (standard error):  
0.008 0.079\n fractal dimension (standard error): 0.001 0.03\n rad  
ius (worst): 7.93 36.04\n texture (worst):  
12.02 49.54\n perimeter (worst): 50.41 251.2\n ar  
ea (worst): 185.2 4254.0\n smoothness (worst):  
0.071 0.223\n compactness (worst): 0.027 1.058\n co  
ncavity (worst): 0.0 1.252\n concave points (wors  
t): 0.0 0.291\n symmetry (worst): 0.  
156 0.664\n fractal dimension (worst): 0.055 0.208\n ==  
===== :Missing Attribute Va  
lues: None\n\n :Class Distribution: 212 - Malignant, 357 - Benign\n\n  
:Creator: Dr. William H. Wolberg, W. Nick Street, Olvi L. Mangasarian\n\n  
:Donor: Nick Street\n\n :Date: November, 1995\n\nThis is a copy of UCI ML  
Breast Cancer Wisconsin (Diagnostic) datasets.\n<https://goo.gl/U2Uwz2>\nFea  
tures are computed from a digitized image of a fine needle\naspirate (FNA) o  
f a breast mass. They describe\ncharacteristics of the cell nuclei present  
in the image.\n\nSeparating plane described above was obtained using\nMultis  
urface Method-Tree (MSM-T) [K. P. Bennett, "Decision Tree\nConstruction Via  
Linear Programming." Proceedings of the 4th\nMidwest Artificial Intelligence  
and Cognitive Science Society,\npp. 97-101, 1992], a classification method w  
hich uses linear\nprogramming to construct a decision tree. Relevant featur  
es\nwere selected using an exhaustive search in the space of 1-4\nfeatures a  
nd 1-3 separating planes.\n\nThe actual linear program used to obtain the se  
parating plane\nin the 3-dimensional space is that described in:\n[K. P. Ben  
nett and O. L. Mangasarian: "Robust Linear\nProgramming Discrimination of Tw  
o Linearly Inseparable Sets",\nOptimization Methods and Software 1, 1992, 23  
-34].\n\nThis database is also available through the UW CS ftp server:\n\n  
p ftp.cs.wisc.edu\ncd math-prog/cpo-dataset/machine-learn/WDBC/\n..\n  
c:: References\n\n - W.N. Street, W.H. Wolberg and O.L. Mangasarian. Nucle  
ar feature extraction \n for breast tumor diagnosis. IS&T/SPIE 1993 Inte  
rnational Symposium on \n Electronic Imaging: Science and Technology, vo  
lume 1905, pages 861-870,\n San Jose, CA, 1993.\n - O.L. Mangasarian,  
W.N. Street and W.H. Wolberg. Breast cancer diagnosis and \n prognosis v  
ia linear programming. Operations Research, 43(4), pages 570-577, \n Jul  
y-August 1995.\n - W.H. Wolberg, W.N. Street, and O.L. Mangasarian. Machin  
e learning techniques\n to diagnose breast cancer from fine-needle aspir  
ates. Cancer Letters 77 (1994) \n 163-171.',  
'feature\_names': array(['mean radius', 'mean texture', 'mean perimeter', 'm  
ean area',  
'mean smoothness', 'mean compactness', 'mean concavity',  
'mean concave points', 'mean symmetry', 'mean fractal dimension',

```
'radius error', 'texture error', 'perimeter error', 'area error',
'smoothness error', 'compactness error', 'concavity error',
'concave points error', 'symmetry error',
'fractal dimension error', 'worst radius', 'worst texture',
'worst perimeter', 'worst area', 'worst smoothness',
'worst compactness', 'worst concavity', 'worst concave points',
'worst symmetry', 'worst fractal dimension'], dtype='<U23'),
'filename': '/Users/ssahu/anaconda3.8.3_2020.07_cf/lib/python3.8/site-packages/sklearn/datasets/data/breast_cancer.csv'}
```

In [3]:

```
print(data.DESCR)
```

```
.. _breast_cancer_dataset:
```

Breast cancer wisconsin (diagnostic) dataset

\*\*Data Set Characteristics:\*\*

:Number of Instances: 569

:Number of Attributes: 30 numeric, predictive attributes and the class

:Attribute Information:  
- radius (mean of distances from center to points on the perimeter)  
- texture (standard deviation of gray-scale values)  
- perimeter  
- area  
- smoothness (local variation in radius lengths)

In [4]:

```
print(type(data['data']))
print(type(data['target']))
```

```
<class 'numpy.ndarray'>
<class 'numpy.ndarray'>
```

In [5]:

```
print(data['data'].shape)
print(data['target'].shape)
print(data['target'][data['target']==0].shape)
print(data['target'][data['target']==1].shape)
```

```
(569, 30)
(569,)
(212,)
(357,)
```

In [6]:

```
df = pd.DataFrame(data.data, columns=data.feature_names)
df
```

Out[6]:

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry	me frac dimensi
0	17.990	10.38	122.80	1001.0	0.11840	0.27760	0.300100	0.147100	0.2419	0.078
1	20.570	17.77	132.90	1326.0	0.08474	0.07864	0.086900	0.070170	0.1812	0.056
2	19.690	21.25	130.00	1203.0	0.10960	0.15990	0.197400	0.127900	0.2069	0.059
3	11.420	20.38	77.58	386.1	0.14250	0.28390	0.241400	0.105200	0.2597	0.097
4	20.290	14.34	135.10	1297.0	0.10030	0.13280	0.198000	0.104300	0.1809	0.058
5	12.450	15.70	82.57	477.1	0.12780	0.17000	0.157800	0.080890	0.2087	0.076
6	18.250	19.98	119.60	1040.0	0.09463	0.10900	0.112700	0.074000	0.1794	0.057
7	13.710	20.83	90.20	577.9	0.11890	0.16450	0.093660	0.059850	0.2196	0.074
8	13.000	21.82	87.50	519.8	0.12730	0.19320	0.185900	0.093530	0.2350	0.073

In [7]:

```
df['CANCER'] = data.target
df
```

Out[7]:

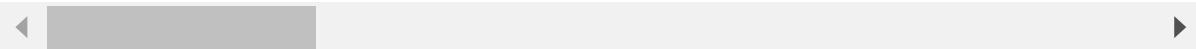
	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry	me frac dimensi
0	17.990	10.38	122.80	1001.0	0.11840	0.27760	0.300100	0.147100	0.2419	0.078
1	20.570	17.77	132.90	1326.0	0.08474	0.07864	0.086900	0.070170	0.1812	0.056
2	19.690	21.25	130.00	1203.0	0.10960	0.15990	0.197400	0.127900	0.2069	0.059
3	11.420	20.38	77.58	386.1	0.14250	0.28390	0.241400	0.105200	0.2597	0.097
4	20.290	14.34	135.10	1297.0	0.10030	0.13280	0.198000	0.104300	0.1809	0.058
5	12.450	15.70	82.57	477.1	0.12780	0.17000	0.157800	0.080890	0.2087	0.076
6	18.250	19.98	119.60	1040.0	0.09463	0.10900	0.112700	0.074000	0.1794	0.057
7	13.710	20.83	90.20	577.9	0.11890	0.16450	0.093660	0.059850	0.2196	0.074
8	13.000	21.82	87.50	519.8	0.12730	0.19320	0.185900	0.093530	0.2350	0.073

In [8]:

```
df.describe(include='all')
```

Out[8]:

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity
<b>count</b>	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000
<b>mean</b>	14.127292	19.289649	91.969033	654.889104	0.096360	0.104341	0.088799
<b>std</b>	3.524049	4.301036	24.298981	351.914129	0.014064	0.052813	0.079720
<b>min</b>	6.981000	9.710000	43.790000	143.500000	0.052630	0.019380	0.000000
<b>25%</b>	11.700000	16.170000	75.170000	420.300000	0.086370	0.064920	0.029560
<b>50%</b>	13.370000	18.840000	86.240000	551.100000	0.095870	0.092630	0.061540
<b>75%</b>	15.780000	21.800000	104.100000	782.700000	0.105300	0.130400	0.130700
<b>max</b>	28.110000	39.280000	188.500000	2501.000000	0.163400	0.345400	0.426800



In [9]:

df.info()

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 569 entries, 0 to 568
Data columns (total 31 columns):
 #   Column           Non-Null Count  Dtype  
--- 
 0   mean radius      569 non-null    float64
 1   mean texture     569 non-null    float64
 2   mean perimeter   569 non-null    float64
 3   mean area        569 non-null    float64
 4   mean smoothness  569 non-null    float64
 5   mean compactness 569 non-null    float64
 6   mean concavity   569 non-null    float64
 7   mean concave points 569 non-null  float64
 8   mean symmetry    569 non-null    float64
 9   mean fractal dimension 569 non-null  float64
 10  radius error    569 non-null    float64
 11  texture error   569 non-null    float64
 12  perimeter error 569 non-null    float64
 13  area error      569 non-null    float64
 14  smoothness error 569 non-null    float64
 15  compactness error 569 non-null    float64
 16  concavity error  569 non-null    float64
 17  concave points error 569 non-null  float64
 18  symmetry error   569 non-null    float64
 19  fractal dimension error 569 non-null  float64
 20  worst radius     569 non-null    float64
 21  worst texture    569 non-null    float64
 22  worst perimeter   569 non-null    float64
 23  worst area        569 non-null    float64
 24  worst smoothness  569 non-null    float64
 25  worst compactness 569 non-null    float64
 26  worst concavity   569 non-null    float64
 27  worst concave points 569 non-null  float64
 28  worst symmetry    569 non-null    float64
 29  worst fractal dimension 569 non-null  float64
 30  CANCER          569 non-null    int64 
dtypes: float64(30), int64(1)
memory usage: 137.9 KB
```

In [10]:

# Correlation

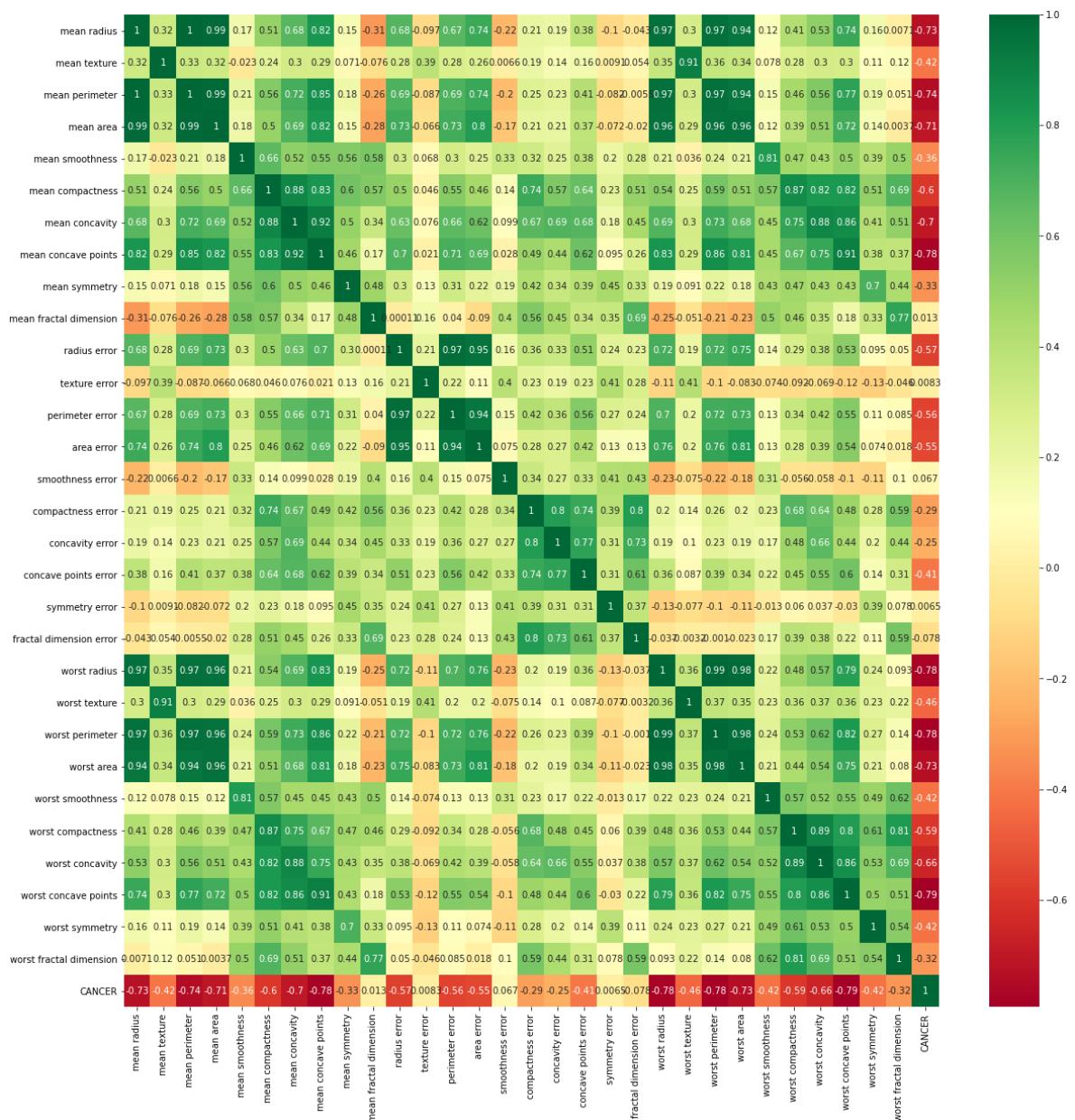
```
import seaborn as sns
import matplotlib.pyplot as plt

# get correlations of each pair of features in the data
corrmat = df.corr()
top_corr_features = corrmat.index
plt.figure(figsize=(20, 20))

# plot heat map
sns.heatmap(df[top_corr_features].corr(), annot=True, cmap="RdYlGn")
```

Out[10]:

&lt;matplotlib.axes.\_subplots.AxesSubplot at 0x119f2b850&gt;



In [11]:

```
X, y = df.iloc[:, :-1], df.iloc[:, -1]
```

In [12]:

```
print(X.shape)
print(y.shape)
```

```
(569, 30)
(569,)
```

In [13]:

```
from sklearn import model_selection

X_train, X_test, y_train, y_test = model_selection.train_test_split(X,
                                                                    y,
                                                                    test_size=0.2,
                                                                    stratify=y,
                                                                    shuffle=True,
                                                                    random_state=0)

print(y.shape[0])
print(y_train.shape[0])
print(y_test.shape[0])
```

```
569
455
114
```

In [14]:

```
print(y_train.shape[0])
print(y_train[y_train==0].shape)
print(y_train[y_train==1].shape)
```

```
455
(170,)
(285,)
```

In [15]:

```
print(y_test.shape[0])
print(y_test[y_test==0].shape)
print(y_test[y_test==1].shape)
```

114  
(42,)  
(72,)

In [16]:

```
import xgboost as xgb
from sklearn import metrics

xgclf = xgb.XGBClassifier()

xgclf.fit(X_train, y_train)
```

Out[16]:

```
XGBClassifier(base_score=0.5, booster='gbtree', colsample_bylevel=1,
              colsample_bynode=1, colsample_bytree=1, gamma=0, gpu_id=-1,
              importance_type='gain', interaction_constraints='',
              learning_rate=0.300000012, max_delta_step=0, max_depth=6,
              min_child_weight=1, missing=nan, monotone_constraints='()',
              n_estimators=100, n_jobs=0, num_parallel_tree=1, random_state=
1,
              reg_alpha=0, reg_lambda=1, scale_pos_weight=1, subsample=1,
              tree_method='exact', validate_parameters=1, verbosity=None)
```

In [17]:

```
print('AUC on train data by XGBoost =', metrics.roc_auc_score(y_true=y_train,
                                                               y_score=xgclf.predict_proba(X_
```

AUC on train data by XGBoost = 1.0

In [18]:

```
print('AUC on test data by XGBoost =', metrics.roc_auc_score(y_true=y_test,
                                                               y_score=xgclf.predict_proba(X_
```

AUC on test data by XGBoost = 0.9887566137566137

In [19]:

```
xgb_model = xgb.XGBClassifier()

# Default-Run of default-hyperparameters
parameters = {'learning_rate': [0.3],
              'max_depth': [6],
              'min_child_weight': [1],
              'n_estimators': [100]}

scorer = metrics.make_scorer(metrics.roc_auc_score,
                             greater_is_better=True,
                             needs_proba=True,
                             needs_threshold=False)

clf_xgb = model_selection.GridSearchCV(estimator=xgb_model,
                                         param_grid=parameters,
                                         n_jobs=-1,
                                         cv=3,
                                         scoring=scorer,
                                         refit=True)

clf_xgb.fit(X_train, y_train)
```

Out[19]:

```
GridSearchCV(cv=3,
             estimator=XGBClassifier(base_score=None, booster=None,
                                      colsample_bylevel=None,
                                      colsample_bynode=None,
                                      colsample_bytree=None, gamma=None,
                                      gpu_id=None, importance_type='gain',
                                      interaction_constraints=None,
                                      learning_rate=None, max_delta_step=None,
                                      max_depth=None, min_child_weight=None,
                                      missing=nan, monotone_constraints=None,
                                      n_estimators=100, n_jobs=None,
                                      num_parallel_tree=None, random_state=None,
                                      reg_alpha=None, reg_lambda=None,
                                      scale_pos_weight=None, subsample=None,
                                      tree_method=None, validate_parameters=None,
                                      verbosity=None),
             n_jobs=-1,
             param_grid={'learning_rate': [0.3], 'max_depth': [6],
                         'min_child_weight': [1], 'n_estimators': [100]},
             scoring=make_scorer(roc_auc_score, needs_proba=True))
```

In [20]:

```
print(clf_xgb.best_params_)
print(clf_xgb.best_score_)
print(clf_xgb.best_estimator_)

{'learning_rate': 0.3, 'max_depth': 6, 'min_child_weight': 1, 'n_estimators': 100}
0.991775491359979
XGBClassifier(base_score=0.5, booster='gbtree', colsample_bylevel=1,
              colsample_bynode=1, colsample_bytree=1, gamma=0, gpu_id=-1,
              importance_type='gain', interaction_constraints='',
              learning_rate=0.3, max_delta_step=0, max_depth=6,
              min_child_weight=1, missing=nan, monotone_constraints='()',
              n_estimators=100, n_jobs=0, num_parallel_tree=1, random_state=
0,
              reg_alpha=0, reg_lambda=1, scale_pos_weight=1, subsample=1,
              tree_method='exact', validate_parameters=1, verbosity=None)
```

In [21]:

```
# 1st-Run for best hyperparameters
parameters = {'learning_rate': [0.1, 0.2, 0.3, 0.4, 0.5],
              'max_depth': [2, 4, 6, 8, 10],
              'min_child_weight': [3, 7, 11, 19, 25],
              'n_estimators': [50, 100, 150, 200, 300, 500]}

scorer = metrics.make_scorer(metrics.roc_auc_score,
                             greater_is_better=True,
                             needs_proba=True,
                             needs_threshold=False)

clf_xgb = model_selection.GridSearchCV(estimator=xgb_model,
                                         param_grid=parameters,
                                         n_jobs=-1,
                                         cv=3,
                                         scoring=scorer,
                                         refit=True)

clf_xgb.fit(X_train, y_train)
```

Out[21]:

```
GridSearchCV(cv=3,
             estimator=XGBClassifier(base_score=None, booster=None,
                                      colsample_bylevel=None,
                                      colsample_bynode=None,
                                      colsample_bytree=None, gamma=None,
                                      gpu_id=None, importance_type='gain',
                                      interaction_constraints=None,
                                      learning_rate=None, max_delta_step=None,
                                      max_depth=None, min_child_weight=None,
                                      missing=nan, monotone_constraints=None,
                                      n_estimators=100, n_jobs...,
                                      num_parallel_tree=None, random_state=None,
                                      reg_alpha=None, reg_lambda=None,
                                      scale_pos_weight=None, subsample=None,
                                      tree_method=None, validate_parameters=None,
                                      verbosity=None),
             n_jobs=-1,
             param_grid={'learning_rate': [0.1, 0.2, 0.3, 0.4, 0.5],
                         'max_depth': [2, 4, 6, 8, 10],
                         'min_child_weight': [3, 7, 11, 19, 25],
                         'n_estimators': [50, 100, 150, 200, 300, 500]},
             scoring=make_scorer(roc_auc_score, needs_proba=True))
```

In [22]:

```
print(clf_xgb.best_params_)
print(clf_xgb.best_score_)
print(clf_xgb.best_estimator_)

{'learning_rate': 0.2, 'max_depth': 4, 'min_child_weight': 3, 'n_estimators': 100}
0.9915842237171878
XGBClassifier(base_score=0.5, booster='gbtree', colsample_bylevel=1,
              colsample_bynode=1, colsample_bytree=1, gamma=0, gpu_id=-1,
              importance_type='gain', interaction_constraints='',
              learning_rate=0.2, max_delta_step=0, max_depth=4,
              min_child_weight=3, missing=nan, monotone_constraints='()', n_estimators=100, n_jobs=0, num_parallel_tree=1, random_state=0,
              reg_alpha=0, reg_lambda=1, scale_pos_weight=1, subsample=1, tree_method='exact', validate_parameters=1, verbosity=None)
```

In [23]:

```
final_model = xgb.XGBClassifier(learning_rate=0.3,
                                  max_depth=6,
                                  min_child_weight=1,
                                  n_estimators=100)

final_model.fit(X_train, y_train)
print('AUC on train data by XGBoost =', metrics.roc_auc_score(y_true=y_train,
                                                               y_score=final_model.predict_proba(X_train)))

print('AUC on test data by XGBoost =', metrics.roc_auc_score(y_true=y_test,
                                                               y_score=final_model.predict_proba(X_test)))
```

AUC on train data by XGBoost = 1.0  
AUC on test data by XGBoost = 0.9887566137566137

# Hyperparameter Optimization For XGBoost using GridSearchCV

In [1]:

```
import numpy as np
import pandas as pd
from sklearn.datasets import load_boston

pd.set_option('display.max_columns', None)
pd.set_option('display.max_rows', None)
```

In [2]:

# Read the Dataset

```
data = load_boston()  
data
```

Out[2]:

```
{'data': array([[6.3200e-03, 1.8000e+01, 2.3100e+00, ..., 1.5300e+01, 3.9690  
e+02,  
    4.9800e+00],  
   [2.7310e-02, 0.0000e+00, 7.0700e+00, ..., 1.7800e+01, 3.9690e+02,  
    9.1400e+00],  
   [2.7290e-02, 0.0000e+00, 7.0700e+00, ..., 1.7800e+01, 3.9283e+02,  
    4.0300e+00],  
   ...,  
   [6.0760e-02, 0.0000e+00, 1.1930e+01, ..., 2.1000e+01, 3.9690e+02,  
    5.6400e+00],  
   [1.0959e-01, 0.0000e+00, 1.1930e+01, ..., 2.1000e+01, 3.9345e+02,  
    6.4800e+00],  
   [4.7410e-02, 0.0000e+00, 1.1930e+01, ..., 2.1000e+01, 3.9690e+02,  
    7.8800e+00]]),  
'target': array([24. , 21.6, 34.7, 33.4, 36.2, 28.7, 22.9, 27.1, 16.5, 18.  
9, 15. ,  
    18.9, 21.7, 20.4, 18.2, 19.9, 23.1, 17.5, 20.2, 18.2, 13.6, 19.6,  
    15.2, 14.5, 15.6, 13.9, 16.6, 14.8, 18.4, 21. , 12.7, 14.5, 13.2,  
    13.1, 13.5, 18.9, 20. , 21. , 24.7, 30.8, 34.9, 26.6, 25.3, 24.7,  
    21.2, 19.3, 20. , 16.6, 14.4, 19.4, 19.7, 20.5, 25. , 23.4, 18.9,  
    35.4, 24.7, 31.6, 23.3, 19.6, 18.7, 16. , 22.2, 25. , 33. , 23.5,  
    19.4, 22. , 17.4, 20.9, 24.2, 21.7, 22.8, 23.4, 24.1, 21.4, 20. ,  
    20.8, 21.2, 20.3, 28. , 23.9, 24.8, 22.9, 23.9, 26.6, 22.5, 22.2,  
    23.6, 28.7, 22.6, 22. , 22.9, 25. , 20.6, 28.4, 21.4, 38.7, 43.8,  
    33.2, 27.5, 26.5, 18.6, 19.3, 20.1, 19.5, 19.5, 20.4, 19.8, 19.4,  
    21.7, 22.8, 18.8, 18.7, 18.5, 18.3, 21.2, 19.2, 20.4, 19.3, 22. ,  
    20.3, 20.5, 17.3, 18.8, 21.4, 15.7, 16.2, 18. , 14.3, 19.2, 19.6,  
    23. , 18.4, 15.6, 18.1, 17.4, 17.1, 13.3, 17.8, 14. , 14.4, 13.4,  
    15.6, 11.8, 13.8, 15.6, 14.6, 17.8, 15.4, 21.5, 19.6, 15.3, 19.4,  
    17. , 15.6, 13.1, 41.3, 24.3, 23.3, 27. , 50. , 50. , 50. , 22.7,  
    25. , 50. , 23.8, 23.8, 22.3, 17.4, 19.1, 23.1, 23.6, 22.6, 29.4,  
    23.2, 24.6, 29.9, 37.2, 39.8, 36.2, 37.9, 32.5, 26.4, 29.6, 50. ,  
    32. , 29.8, 34.9, 37. , 30.5, 36.4, 31.1, 29.1, 50. , 33.3, 30.3,  
    34.6, 34.9, 32.9, 24.1, 42.3, 48.5, 50. , 22.6, 24.4, 22.5, 24.4,  
    20. , 21.7, 19.3, 22.4, 28.1, 23.7, 25. , 23.3, 28.7, 21.5, 23. ,  
    26.7, 21.7, 27.5, 30.1, 44.8, 50. , 37.6, 31.6, 46.7, 31.5, 24.3,  
    31.7, 41.7, 48.3, 29. , 24. , 25.1, 31.5, 23.7, 23.3, 22. , 20.1,  
    22.2, 23.7, 17.6, 18.5, 24.3, 20.5, 24.5, 26.2, 24.4, 24.8, 29.6,  
    42.8, 21.9, 20.9, 44. , 50. , 36. , 30.1, 33.8, 43.1, 48.8, 31. ,  
    36.5, 22.8, 30.7, 50. , 43.5, 20.7, 21.1, 25.2, 24.4, 35.2, 32.4,  
    32. , 33.2, 33.1, 29.1, 35.1, 45.4, 35.4, 46. , 50. , 32.2, 22. ,  
    20.1, 23.2, 22.3, 24.8, 28.5, 37.3, 27.9, 23.9, 21.7, 28.6, 27.1,  
    20.3, 22.5, 29. , 24.8, 22. , 26.4, 33.1, 36.1, 28.4, 33.4, 28.2,  
    22.8, 20.3, 16.1, 22.1, 19.4, 21.6, 23.8, 16.2, 17.8, 19.8, 23.1,  
    21. , 23.8, 23.1, 20.4, 18.5, 25. , 24.6, 23. , 22.2, 19.3, 22.6,  
    19.8, 17.1, 19.4, 22.2, 20.7, 21.1, 19.5, 18.5, 20.6, 19. , 18.7,  
    32.7, 16.5, 23.9, 31.2, 17.5, 17.2, 23.1, 24.5, 26.6, 22.9, 24.1,  
    18.6, 30.1, 18.2, 20.6, 17.8, 21.7, 22.7, 22.6, 25. , 19.9, 20.8,  
    16.8, 21.9, 27.5, 21.9, 23.1, 50. , 50. , 50. , 50. , 13.8,  
    13.8, 15. , 13.9, 13.3, 13.1, 10.2, 10.4, 10.9, 11.3, 12.3, 8.8,  
    7.2, 10.5, 7.4, 10.2, 11.5, 15.1, 23.2, 9.7, 13.8, 12.7, 13.1,  
    12.5, 8.5, 5. , 6.3, 5.6, 7.2, 12.1, 8.3, 8.5, 5. , 11.9,
```

```
27.9, 17.2, 27.5, 15. , 17.2, 17.9, 16.3, 7. , 7.2, 7.5, 10.4,
8.8, 8.4, 16.7, 14.2, 20.8, 13.4, 11.7, 8.3, 10.2, 10.9, 11. ,
9.5, 14.5, 14.1, 16.1, 14.3, 11.7, 13.4, 9.6, 8.7, 8.4, 12.8,
10.5, 17.1, 18.4, 15.4, 10.8, 11.8, 14.9, 12.6, 14.1, 13. , 13.4,
15.2, 16.1, 17.8, 14.9, 14.1, 12.7, 13.5, 14.9, 20. , 16.4, 17.7,
19.5, 20.2, 21.4, 19.9, 19. , 19.1, 19.1, 20.1, 19.9, 19.6, 23.2,
29.8, 13.8, 13.3, 16.7, 12. , 14.6, 21.4, 23. , 23.7, 25. , 21.8,
20.6, 21.2, 19.1, 20.6, 15.2, 7. , 8.1, 13.6, 20.1, 21.8, 24.5,
23.1, 19.7, 18.3, 21.2, 17.5, 16.8, 22.4, 20.6, 23.9, 22. , 11.9]),
'feature_names': array(['CRIM', 'ZN', 'INDUS', 'CHAS', 'NOX', 'RM', 'AGE',
'DIS', 'RAD',
'TAX', 'PTRATIO', 'B', 'LSTAT'], dtype='<U7'),
'DESCR': "... _boston_dataset:\n\nBoston house prices dataset\n-----\n-----\n**Data Set Characteristics:** \n\n :Number of Instances: 506 \n\n :Number of Attributes: 13 numeric/categorical predictive. Median Value (attribute 14) is usually the target.\n\n :Attribute Information (in order):\n      - CRIM    per capita crime rate by town\n      - Z        proportion of residential land zoned for lots over 25,000 sq.ft.\n      - INDUS   proportion of non-retail business acres per town\n      - CHAS    Charles River dummy variable (= 1 if tract bounds river; 0 otherwise)\n      - NOX     nitric oxides concentration (parts per 10 million)\n      - RM      average number of rooms per dwelling\n      - AGE     proportion of owner-occupied units built prior to 1940\n      - DIS     weighted distances to five Boston employment centres\n      - RAD     index of accessibility to radial highways\n      - TAX     full-value property-tax rate per $10,000\n      - PTRATIO pupil-teacher ratio by town\n      - B       1000(Bk - 0.63)^2 where Bk is the proportion of blacks by town\n      - LSTAT   % lower status of the population\n      - MEDV    Median value of owner-occupied homes in $1000's\n\n :Missing Attribute Values: None\n\n :Creator: Harrison, D. and Rubinfeld, D.L.\n\nThis is a copy of UCI ML housing dataset.\nhttps://archive.ics.uci.edu/ml/machine-learning-databases/housing/\n\nThis dataset was taken from the StatLib library which is maintained at Carnegie Mellon University.\n\nThe Boston house-price data of Harrison, D. and Rubinfeld, D.L. 'Hedonic\nprices and the demand for clean air', J. Environmental Economics & Management, vol.5, 81-102, 1978. Used in Belsley, Kuh & Welsch, 'Regression diagnostics\n...', Wiley, 1980. N.B. Various transformations are used in the table on pages 244-261 of the latter.\n\nThe Boston house-price data has been used in many machine learning papers that address regression\nproblems.\n.. topic:: References\n - Belsley, Kuh & Welsch, 'Regression diagnostics: Identifying Influential Data and Sources of Collinearity', Wiley, 1980. 244-261.\n - Quinlan,R. (1993). Combining Instance-Based and Model-Based Learning. In Proceedings on the Tenth International Conference of Machine Learning, 236-243, University of Massachusetts, Amherst. Morgan Kaufmann.\n",
'filename': '/Users/ssahu/anaconda3.8.3_2020.07_cf/lib/python3.8/site-packages/sklearn/datasets/data/boston_house_prices.csv'}
```

In [3]:

```
print(data.DESCR)
```

```
.. _boston_dataset:
```

```
Boston house prices dataset
```

```
-----
```

```
**Data Set Characteristics:**
```

```
:Number of Instances: 506
```

```
:Number of Attributes: 13 numeric/categorical predictive. Median Value (attribute 14) is usually the target.
```

```
:Attribute Information (in order):
```

```
- CRIM per capita crime rate by town  
- ZN proportion of residential land zoned for lots over 25,000 sq.ft.  
- INDUS proportion of non-retail business acres per town  
- CHAS Charles River dummy variable (= 1 if tract bounds river; 0 otherwise)  
- NOX nitric oxides concentration (parts per 10 million)  
- RM average number of rooms per dwelling  
- AGE proportion of owner-occupied units built prior to 1940  
- DIS weighted distances to five Boston employment centres  
- RAD index of accessibility to radial highways  
- TAX full-value property-tax rate per $10,000  
- PTRATIO pupil-teacher ratio by town  
- B  $1000(Bk - 0.63)^2$  where Bk is the proportion of blacks by town  
- LSTAT % lower status of the population  
- MEDV Median value of owner-occupied homes in $1000's
```

```
:Missing Attribute Values: None
```

```
:Creator: Harrison, D. and Rubinfeld, D.L.
```

This is a copy of UCI ML housing dataset.

<https://archive.ics.uci.edu/ml/machine-learning-databases/housing/> (<http://archive.ics.uci.edu/ml/machine-learning-databases/housing/>)

This dataset was taken from the StatLib library which is maintained at Carnegie Mellon University.

The Boston house-price data of Harrison, D. and Rubinfeld, D.L. 'Hedonic prices and the demand for clean air', J. Environ. Economics & Management, vol.5, 81-102, 1978. Used in Belsley, Kuh & Welsch, 'Regression diagnostics ...', Wiley, 1980. N.B. Various transformations are used in the table on pages 244-261 of the latter.

The Boston house-price data has been used in many machine learning papers that address regression problems.

```
.. topic:: References
```

- Belsley, Kuh & Welsch, 'Regression diagnostics: Identifying Influential Data and Sources of Collinearity', Wiley, 1980. 244-261.
- Quinlan,R. (1993). Combining Instance-Based and Model-Based Learning. In Proceedings on the Tenth International Conference of Machine Learning, 236-243, University of Massachusetts, Amherst. Morgan Kaufmann.

In [4]:

```
print(type(data['data']))
print(type(data['target']))
```

```
<class 'numpy.ndarray'>
<class 'numpy.ndarray'>
```

In [5]:

```
print(data['data'].shape)
print(data['target'].shape)
```

```
(506, 13)
(506,)
```

In [6]:

```
df = pd.DataFrame(data.data, columns=data.feature_names)
df
```

Out[6]:

	CRIM	ZN	INDUS	CHAS	NOX	RM	AGE	DIS	RAD	TAX	PTRATIO	B	LSTAT
0	0.00632	18.0	2.31	0.0	0.5380	6.575	65.2	4.0900	1.0	296.0	15.3	396.90	4.98
1	0.02731	0.0	7.07	0.0	0.4690	6.421	78.9	4.9671	2.0	242.0	17.8	396.90	9.14
2	0.02729	0.0	7.07	0.0	0.4690	7.185	61.1	4.9671	2.0	242.0	17.8	392.83	4.03
3	0.03237	0.0	2.18	0.0	0.4580	6.998	45.8	6.0622	3.0	222.0	18.7	394.63	2.94
4	0.06905	0.0	2.18	0.0	0.4580	7.147	54.2	6.0622	3.0	222.0	18.7	396.90	5.33
5	0.02985	0.0	2.18	0.0	0.4580	6.430	58.7	6.0622	3.0	222.0	18.7	394.12	5.21
6	0.08829	12.5	7.87	0.0	0.5240	6.012	66.6	5.5605	5.0	311.0	15.2	395.60	12.43
7	0.14455	12.5	7.87	0.0	0.5240	6.172	96.1	5.9505	5.0	311.0	15.2	396.90	19.15
8	0.21124	12.5	7.87	0.0	0.5240	5.631	100.0	6.0821	5.0	311.0	15.2	386.63	29.93
9	0.17004	12.5	7.87	0.0	0.5240	6.004	85.9	6.5921	5.0	311.0	15.2	386.71	17.10
10	0.22489	12.5	7.87	0.0	0.5240	6.377	94.3	6.3467	5.0	311.0	15.2	392.52	20.45

In [7]:

```
df['PRICE'] = data.target
df
```

Out[7]:

	CRIM	ZN	INDUS	CHAS	NOX	RM	AGE	DIS	RAD	TAX	PTRATIO	B	LSTAT
0	0.00632	18.0	2.31	0.0	0.5380	6.575	65.2	4.0900	1.0	296.0	15.3	396.90	4.98
1	0.02731	0.0	7.07	0.0	0.4690	6.421	78.9	4.9671	2.0	242.0	17.8	396.90	9.14
2	0.02729	0.0	7.07	0.0	0.4690	7.185	61.1	4.9671	2.0	242.0	17.8	392.83	4.03
3	0.03237	0.0	2.18	0.0	0.4580	6.998	45.8	6.0622	3.0	222.0	18.7	394.63	2.94
4	0.06905	0.0	2.18	0.0	0.4580	7.147	54.2	6.0622	3.0	222.0	18.7	396.90	5.33
5	0.02985	0.0	2.18	0.0	0.4580	6.430	58.7	6.0622	3.0	222.0	18.7	394.12	5.21
6	0.08829	12.5	7.87	0.0	0.5240	6.012	66.6	5.5605	5.0	311.0	15.2	395.60	12.43
7	0.14455	12.5	7.87	0.0	0.5240	6.172	96.1	5.9505	5.0	311.0	15.2	396.90	19.15
8	0.21124	12.5	7.87	0.0	0.5240	5.631	100.0	6.0821	5.0	311.0	15.2	386.63	29.93
9	0.17004	12.5	7.87	0.0	0.5240	6.004	85.9	6.5921	5.0	311.0	15.2	386.71	17.10

In [8]:

```
df.describe(include='all')
```

Out[8]:

	CRIM	ZN	INDUS	CHAS	NOX	RM	AGE	
count	506.000000	506.000000	506.000000	506.000000	506.000000	506.000000	506.000000	50
mean	3.613524	11.363636	11.136779	0.069170	0.554695	6.284634	68.574901	
std	8.601545	23.322453	6.860353	0.253994	0.115878	0.702617	28.148861	
min	0.006320	0.000000	0.460000	0.000000	0.385000	3.561000	2.900000	
25%	0.082045	0.000000	5.190000	0.000000	0.449000	5.885500	45.025000	
50%	0.256510	0.000000	9.690000	0.000000	0.538000	6.208500	77.500000	
75%	3.677083	12.500000	18.100000	0.000000	0.624000	6.623500	94.075000	
max	88.976200	100.000000	27.740000	1.000000	0.871000	8.780000	100.000000	100

In [9]:

```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 506 entries, 0 to 505
Data columns (total 14 columns):
 #   Column    Non-Null Count  Dtype  
--- 
 0   CRIM      506 non-null    float64
 1   ZN        506 non-null    float64
 2   INDUS     506 non-null    float64
 3   CHAS      506 non-null    float64
 4   NOX       506 non-null    float64
 5   RM         506 non-null    float64
 6   AGE        506 non-null    float64
 7   DIS        506 non-null    float64
 8   RAD        506 non-null    float64
 9   TAX        506 non-null    float64
 10  PTRATIO   506 non-null    float64
 11  B          506 non-null    float64
 12  LSTAT     506 non-null    float64
 13  PRICE      506 non-null    float64
dtypes: float64(14)
memory usage: 55.5 KB
```

In [10]:

# Correlation

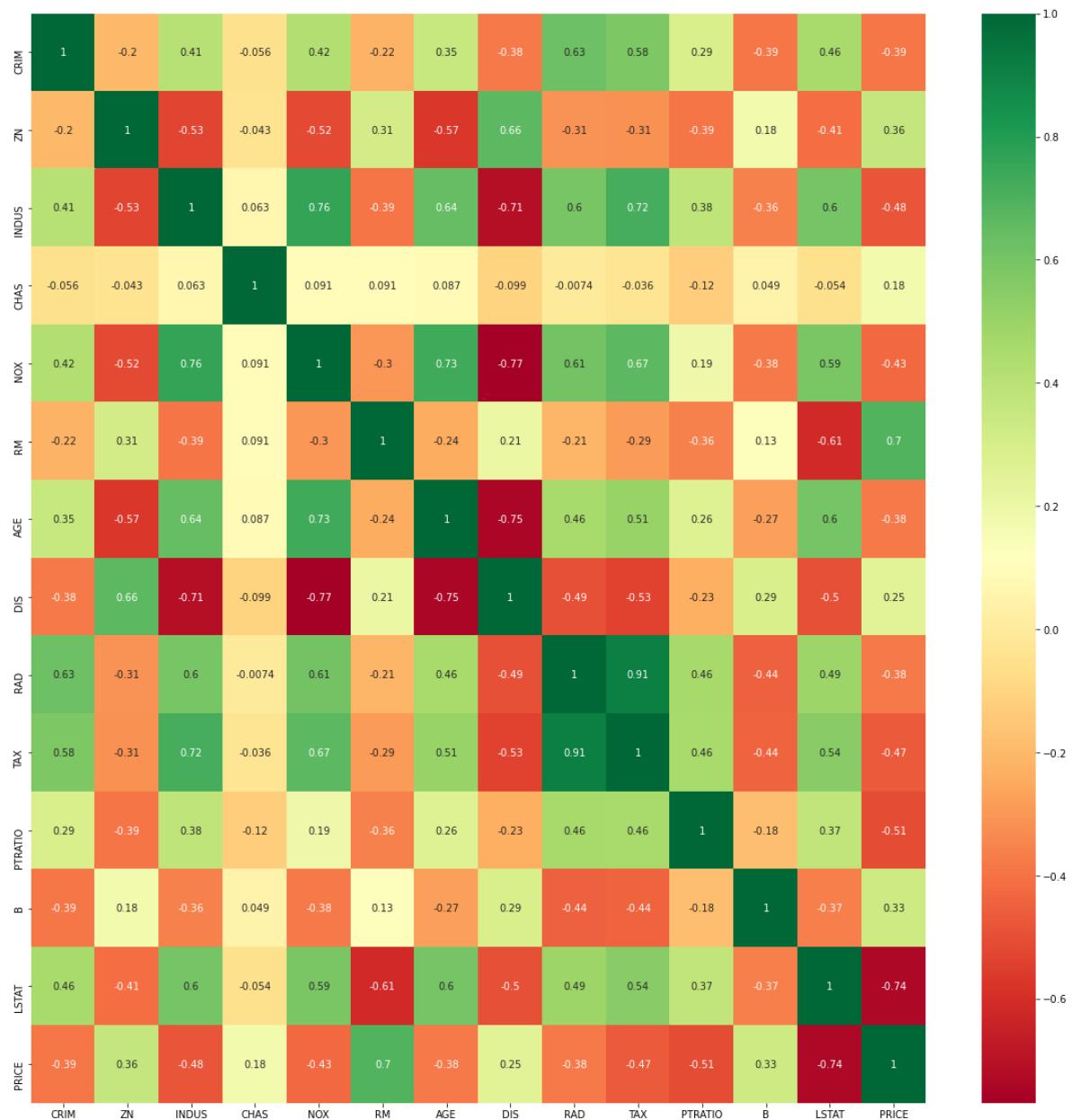
```
import seaborn as sns
import matplotlib.pyplot as plt

#get correlations of each pair of features in the data
corrmat = df.corr()
top_corr_features = corrmat.index
plt.figure(figsize=(20, 20))

#plot heatmap
sns.heatmap(df[top_corr_features].corr(), annot=True, cmap="RdYlGn")
```

Out[10]:

&lt;matplotlib.axes.\_subplots.AxesSubplot at 0x11b830fa0&gt;



In [11]:

```
X, y = df.iloc[:, :-1], df.iloc[:, -1]
```

In [12]:

```
print(X.shape)
print(y.shape)
```

```
(506, 13)
(506,)
```

In [13]:

```
from sklearn import model_selection

X_train, X_test, y_train, y_test = model_selection.train_test_split(X,
                                                                    y,
                                                                    test_size=0.2,
                                                                    shuffle=True,
                                                                    random_state=0)

print(y.shape[0])
print(y_train.shape[0])
print(y_test.shape[0])
```

```
506
404
102
```

In [14]:

```
import xgboost as xgb
xgreg = xgb.XGBRegressor()
xgreg.fit(X_train, y_train)
```

Out[14]:

```
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=1, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints='',
             learning_rate=0.300000012, max_delta_step=0, max_depth=6,
             min_child_weight=1, missing=nan, monotone_constraints='()',
             n_estimators=100, n_jobs=0, num_parallel_tree=1, random_state=
0,
             reg_alpha=0, reg_lambda=1, scale_pos_weight=1, subsample=1,
             tree_method='exact', validate_parameters=1, verbosity=None)
```

In [15]:

```
# r2_score, coefficient of determination
score = xgreg.score(X_train, y_train)
print('r2_score on training data =', score)
```

```
r2_score on training data = 0.9999964964198947
```

In [16]:

```
from sklearn import metrics

print('r2_score on training data =', metrics.r2_score(y_true=y_train,
                                                       y_pred=xgreg.predict(X_train),
                                                       multioutput='variance_weighted'))
```

```
r2_score on training data = 0.9999964964198947
```

In [17]:

```
print('r2_score on test data =', metrics.r2_score(y_true=y_test,
                                                       y_pred=xgreg.predict(X_test),
                                                       multioutput='variance_weighted'))
```

```
r2_score on test data = 0.7375983263596111
```

In [18]:

```
# Hyperparameter Optimization

xgreg = xgb.XGBRegressor()

# Default-Run of default-hyperparameters
parameters = {'learning_rate': [0.3],
               'max_depth': [6],
               'min_child_weight': [1],
               'n_estimators': [100]}

reg_xgb = model_selection.GridSearchCV(estimator=xgreg,
                                         param_grid=parameters,
                                         n_jobs=-1,
                                         cv=3,
                                         refit=True)

reg_xgb.fit(X_train, y_train)
```

Out[18]:

```
GridSearchCV(cv=3,
             estimator=XGBRegressor(base_score=None, booster=None,
                                    colsample_bylevel=None,
                                    colsample_bynode=None,
                                    colsample_bytree=None, gamma=None,
                                    gpu_id=None, importance_type='gain',
                                    interaction_constraints=None,
                                    learning_rate=None, max_delta_step=None,
                                    max_depth=None, min_child_weight=None,
                                    missing=nan, monotone_constraints=None,
                                    n_estimators=100, n_jobs=None,
                                    num_parallel_tree=None, random_state=None,
                                    reg_alpha=None, reg_lambda=None,
                                    scale_pos_weight=None, subsample=None,
                                    tree_method=None, validate_parameters=None,
                                    verbosity=None),
             n_jobs=-1,
             param_grid={'learning_rate': [0.3], 'max_depth': [6],
                         'min_child_weight': [1], 'n_estimators': [100]})
```

In [19]:

```
print(reg_xgb.best_params_)
print(reg_xgb.best_score_)
print(reg_xgb.best_estimator_)

{'learning_rate': 0.3, 'max_depth': 6, 'min_child_weight': 1, 'n_estimators': 100}
0.8265796897665796
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=1, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints='',
             learning_rate=0.3, max_delta_step=0, max_depth=6,
             min_child_weight=1, missing=nan, monotone_constraints='()',
             n_estimators=100, n_jobs=0, num_parallel_tree=1, random_state=
0,
             reg_alpha=0, reg_lambda=1, scale_pos_weight=1, subsample=1,
             tree_method='exact', validate_parameters=1, verbosity=None)
```

In [20]:

```
# 1st-Run for best hyperparameters
parameters = {'learning_rate': [0.1, 0.2, 0.3, 0.4, 0.5],
              'max_depth': [2, 4, 6, 8, 10],
              'min_child_weight': [1, 10, 20, 30, 40, 50],
              'n_estimators': [100, 200, 300, 400, 500]}

reg_xgb = model_selection.GridSearchCV(estimator=xgreg,
                                         param_grid=parameters,
                                         n_jobs=-1,
                                         cv=3,
                                         refit=True)

reg_xgb.fit(X_train, y_train)
```

Out[20]:

```
GridSearchCV(cv=3,
             estimator=XGBRegressor(base_score=None, booster=None,
                                    colsample_bylevel=None,
                                    colsample_bynode=None,
                                    colsample_bytree=None, gamma=None,
                                    gpu_id=None, importance_type='gain',
                                    interaction_constraints=None,
                                    learning_rate=None, max_delta_step=None,
                                    max_depth=None, min_child_weight=None,
                                    missing=nan, monotone_constraints=None,
                                    n_estimators=100, n_jobs=None,
                                    num_parallel_tree=None, random_state=None,
                                    reg_alpha=None, reg_lambda=None,
                                    scale_pos_weight=None, subsample=None,
                                    tree_method=None, validate_parameters=None,
                                    verbosity=None),
             n_jobs=-1,
             param_grid={'learning_rate': [0.1, 0.2, 0.3, 0.4, 0.5],
                         'max_depth': [2, 4, 6, 8, 10],
                         'min_child_weight': [1, 10, 20, 30, 40, 50],
                         'n_estimators': [100, 200, 300, 400, 500]})
```

In [21]:

```
print(reg_xgb.best_params_)
print(reg_xgb.best_score_)
print(reg_xgb.best_estimator_)

{'learning_rate': 0.4, 'max_depth': 4, 'min_child_weight': 20, 'n_estimators': 100}
0.875135968698512
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=1, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints='',
             learning_rate=0.4, max_delta_step=0, max_depth=4,
             min_child_weight=20, missing=nan, monotone_constraints='()',
             n_estimators=100, n_jobs=0, num_parallel_tree=1, random_state=
0,
             reg_alpha=0, reg_lambda=1, scale_pos_weight=1, subsample=1,
             tree_method='exact', validate_parameters=1, verbosity=None)
```

In [22]:

```
# 2nd-Run for best hyperparameters
parameters = {'learning_rate': [0.3, 0.35, 0.4, 0.45, 0.5],
              'max_depth': [2, 3, 4, 5, 6],
              'min_child_weight': [10, 15, 20, 25, 30],
              'n_estimators': [50, 100, 150, 200, 250]}

reg_xgb = model_selection.GridSearchCV(estimator=xgreg,
                                         param_grid=parameters,
                                         n_jobs=-1,
                                         cv=3,
                                         refit=True)

reg_xgb.fit(X_train, y_train)
```

Out[22]:

```
GridSearchCV(cv=3,
             estimator=XGBRegressor(base_score=None, booster=None,
                                    colsample_bylevel=None,
                                    colsample_bynode=None,
                                    colsample_bytree=None, gamma=None,
                                    gpu_id=None, importance_type='gain',
                                    interaction_constraints=None,
                                    learning_rate=None, max_delta_step=None,
                                    max_depth=None, min_child_weight=None,
                                    missing=nan, monotone_constraints=None,
                                    n_estimators=100, n_jobs=None,
                                    num_parallel_tree=None, random_state=None,
                                    reg_alpha=None, reg_lambda=None,
                                    scale_pos_weight=None, subsample=None,
                                    tree_method=None, validate_parameters=None,
                                    verbosity=None),
             n_jobs=-1,
             param_grid={'learning_rate': [0.3, 0.35, 0.4, 0.45, 0.5],
                         'max_depth': [2, 3, 4, 5, 6],
                         'min_child_weight': [10, 15, 20, 25, 30],
                         'n_estimators': [50, 100, 150, 200, 250]})
```

In [23]:

```
print(reg_xgb.best_params_)
print(reg_xgb.best_score_)
print(reg_xgb.best_estimator_)

{'learning_rate': 0.4, 'max_depth': 4, 'min_child_weight': 20, 'n_estimators': 100}
0.875135968698512
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=1, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints='',
             learning_rate=0.4, max_delta_step=0, max_depth=4,
             min_child_weight=20, missing=nan, monotone_constraints='()',
             n_estimators=100, n_jobs=0, num_parallel_tree=1, random_state=
0,
             reg_alpha=0, reg_lambda=1, scale_pos_weight=1, subsample=1,
             tree_method='exact', validate_parameters=1, verbosity=None)
```

In [24]:

```
# 3rd-Run for best hyperparameters
parameters = {'learning_rate': [0.35, 0.375, 0.4, 0.425, 0.45],
              'max_depth': [3, 4, 5, 6, 7],
              'min_child_weight': [15, 18, 20, 22, 25],
              'n_estimators': [80, 90, 100, 110, 120]}

reg_xgb = model_selection.GridSearchCV(estimator=xgreg,
                                         param_grid=parameters,
                                         n_jobs=-1,
                                         cv=3,
                                         refit=True)

reg_xgb.fit(X_train, y_train)
```

Out[24]:

```
GridSearchCV(cv=3,
             estimator=XGBRegressor(base_score=None, booster=None,
                                    colsample_bylevel=None,
                                    colsample_bynode=None,
                                    colsample_bytree=None, gamma=None,
                                    gpu_id=None, importance_type='gain',
                                    interaction_constraints=None,
                                    learning_rate=None, max_delta_step=None,
                                    max_depth=None, min_child_weight=None,
                                    missing=nan, monotone_constraints=None,
                                    n_estimators=100, n_jobs=None,
                                    num_parallel_tree=None, random_state=None,
                                    reg_alpha=None, reg_lambda=None,
                                    scale_pos_weight=None, subsample=None,
                                    tree_method=None, validate_parameters=None,
                                    verbosity=None),
             n_jobs=-1,
             param_grid={'learning_rate': [0.35, 0.375, 0.4, 0.425, 0.45],
                         'max_depth': [3, 4, 5, 6, 7],
                         'min_child_weight': [15, 18, 20, 22, 25],
                         'n_estimators': [80, 90, 100, 110, 120]})
```

In [25]:

```
print(reg_xgb.best_params_)
print(reg_xgb.best_score_)
print(reg_xgb.best_estimator_)

{'learning_rate': 0.425, 'max_depth': 3, 'min_child_weight': 22, 'n_estimators': 120}
0.8779593850474777
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=1, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints='',
             learning_rate=0.425, max_delta_step=0, max_depth=3,
             min_child_weight=22, missing=nan, monotone_constraints='()',
             n_estimators=120, n_jobs=0, num_parallel_tree=1, random_state=
0,
             reg_alpha=0, reg_lambda=1, scale_pos_weight=1, subsample=1,
             tree_method='exact', validate_parameters=1, verbosity=None)
```

In [26]:

```
print('r2_score on test data =', metrics.r2_score(y_true=y_test,
                                                    y_pred=reg_xgb.predict(X_test),
                                                    multioutput='variance_weighted'))
```

r2\_score on test data = 0.7639250257078705

In [27]:

```
final_model = xgb.XGBRegressor(learning_rate=0.425,
                                max_depth=3,
                                min_child_weight=22,
                                n_estimators=120)

final_model.fit(X_train,y_train)
print('r2_score on train data =', metrics.r2_score(y_true=y_train,
                                                    y_pred=reg_xgb.predict(X_train),
                                                    multioutput='variance_weighted'))

print('r2_score on test data =', metrics.r2_score(y_true=y_test,
                                                    y_pred=reg_xgb.predict(X_test),
                                                    multioutput='variance_weighted'))
```

r2\_score on train data = 0.9922625518853955

r2\_score on test data = 0.7639250257078705



# Kaggle Practice Exercise

This is a practice session in which we will solve the Kaggle competition [TalkingData AdTracking Fraud Detection Challenge](#). The training set, as well as the solution, is provided in here. Please implement the code and try tuning the different parameters to achieve a better result, but first, let's understand why it is beneficial to participate in Kaggle competitions.

Note that this is given to you as an exercise by professor Raghavan where you are requested to read the notebook, modify and improvise the code, and optionally participate in the Kaggle competition. A great way to learn from other people on Kaggle is to [read the kernels shared by them](#) and incorporate useful things into your own code.





Please download the following files:

**iPython Notebook****Download****Training data****Download**

**NOTE:** We have used only a fraction of the training set (train\_sample, 100k rows), the full training data on Kaggle (train.csv) has about 180 million rows. For better understanding, you are required to implement the same code on a significant portion of the training dataset.

Hope you have gone through the Notebook. Let's answer the following questions:

**Question 2/3**

Mandatory



## Number of Fits

How many fits do we need to do if we define the param\_grid as follows in a 5-fold crossvalidation?

```
param_grid = {"base_estimator__max_depth": [2, 5],  
             "learning_rate": [0.2, 0.6, 0.9],  
             "subsample": [0.3, 0.6, 0.9]  
             }
```



Navigate

Q&amp;A

 90

Correct

Feedback:

We have  $2*3*3 = 18$  combinations of parameter values. On this, performing a 5-fold cross-validation set  $18*5 = 90$  fits.

 18

Your answer is Correct.

Attempt 2 of 2

Continue

## Additional References

- Installation Guide: XGBoost

Report an error



PREVIOUS

XGBoost Lab

NEXT

Summary





Please download the following files:

**iPython Notebook****Download****Training data****Download**

**NOTE:** We have used only a fraction of the training set (train\_sample, 100k rows), the full training data on Kaggle (train.csv) has about 180 million rows. For better understanding, you are required to implement the same code on a significant portion of the training dataset.

Hope you have gone through the Notebook. Let's answer the following questions:

**Question 3/3**

Mandatory



## Trade Off

We tune learning\_rate and n\_estimators together.

 True

Incorrect

Feedback:

PG Diploma in  
Data Science  
Aug 2020

 Learn

 Live

 Jobs

 Discussions

 Navigate

 Raise

 Correct

 Q&A

 Feedback:

There is a trade-off between learning\_rate and n\_estimators. Hence, we tune only one of them.

Your answer is Wrong.

Attempt 1 of 1

Continue

## Additional References

- Installation Guide: XGBoost

 Report an error



PREVIOUS  
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NEXT  
Summary

# TalkingData: Fraudulent Click Prediction

In this notebook, we will apply various boosting algorithms to solve an interesting classification problem from the domain of 'digital fraud'.

The analysis is divided into the following sections:

- Understanding the business problem
- Understanding and exploring the data
- Feature engineering: Creating new features
- Model building and evaluation: AdaBoost
- Modelling building and evaluation: Gradient Boosting
- Modelling building and evaluation: XGBoost

## Understanding the Business Problem

[TalkingData](https://www.talkingdata.com/) (<https://www.talkingdata.com/>) is a Chinese big data company, and one of their areas of expertise is mobile advertisements.

In mobile advertisements, **click fraud** is a major source of losses. Click fraud is the practice of repeatedly clicking on an advertisement hosted on a website with the intention of generating revenue for the host website or draining revenue from the advertiser.

In this case, TalkingData happens to be serving the advertisers (their clients). TalkingData cover a whopping **approx. 70% of the active mobile devices in China**, of which 90% are potentially fraudulent (i.e. the user is actually not going to download the app after clicking).

You can imagine the amount of money they can help clients save if they are able to predict whether a given click is fraudulent (or equivalently, whether a given click will result in a download).

Their current approach to solve this problem is that they've generated a blacklist of IP addresses - those IPs which produce lots of clicks, but never install any apps. Now, they want to try some advanced techniques to predict the probability of a click being genuine/fraud.

In this problem, we will use the features associated with clicks, such as IP address, operating system, device type, time of click etc. to predict the probability of a click being fraud.

They have released [the problem on Kaggle here.](https://www.kaggle.com/c/talkingdata-adtracking-fraud-detection) (<https://www.kaggle.com/c/talkingdata-adtracking-fraud-detection>).

## Understanding and Exploring the Data

The data contains observations of about 240 million clicks, and whether a given click resulted in a download or not (1/0).

On Kaggle, the data is split into train.csv and train\_sample.csv (100,000 observations). We'll use the smaller train\_sample.csv in this notebook for speed, though while training the model for Kaggle submissions, the full training data will obviously produce better results.

The detailed data dictionary is mentioned here:

- ip : ip address of click.
- app : app id for marketing.
- device : device type id of user mobile phone (e.g., iphone 6 plus, iphone 7, huawei mate 7, etc.)
- os : os version id of user mobile phone
- channel : channel id of mobile ad publisher
- click\_time : timestamp of click (UTC)
- attributed\_time : if user download the app for after clicking an ad, this is the time of the app download
- is\_attributed : the target that is to be predicted, indicating the app was downloaded

Let's try finding some useful trends in the data.

In [135]:

```
import numpy as np
import pandas as pd
import sklearn
import matplotlib.pyplot as plt
import seaborn as sns

from sklearn.cross_validation import train_test_split
from sklearn.model_selection import KFold
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import cross_val_score
from sklearn.preprocessing import LabelEncoder
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import AdaBoostClassifier
from sklearn.ensemble import GradientBoostingClassifier
from sklearn import metrics

import xgboost as xgb
from xgboost import XGBClassifier
from xgboost import plot_importance
import gc # for deleting unused variables
%matplotlib inline

import os
import warnings
warnings.filterwarnings('ignore')
```

## Reading the Data

The code below reads the train\_sample.csv file if you set testing = True, else reads the full train.csv file. You can read the sample while tuning the model etc., and then run the model on the full data once done.

### **Important Note: Save memory when the data is huge**

Since the training data is quite huge, the program will be quite slow if you don't consciously follow some best practices to save memory. This notebook demonstrates some of those practices.

In [3]:

```
# reading training data

# specify column dtypes to save memory (by default pandas reads some columns as floats)
dtypes = {
    'ip' : 'uint16',
    'app' : 'uint16',
    'device' : 'uint16',
    'os' : 'uint16',
    'channel' : 'uint16',
    'is_attributed' : 'uint8',
    'click_id' : 'uint32' # note that click_id is only in test data, not training
}

# read training_sample.csv for quick testing/debug, else read the full train.csv
testing = True
if testing:
    train_path = "train_sample.csv"
    skiprows = None
    nrows = None
    colnames=['ip','app','device','os', 'channel', 'click_time', 'is_attributed']
else:
    train_path = "train.csv"
    skiprows = range(1, 144903891)
    nrows = 10000000
    colnames=['ip','app','device','os', 'channel', 'click_time', 'is_attributed']

# read training data
train_sample = pd.read_csv(train_path, skiprows=skiprows, nrows=nrows, dtype=dtypes, usecol
```

In [4]:

```
# length of training data
len(train_sample.index)
```

Out[4]:

100000

In [9]:

```
# Displays memory consumed by each column ---
print(train_sample.memory_usage())
```

Index	
ip	200000
app	200000
device	200000
os	200000
channel	200000
click_time	800000
is_attributed	100000
dtype:	int64

In [6]:

```
# space used by training data
print('Training dataset uses {0} MB'.format(train_sample.memory_usage().sum()/1024**2))
```

Training dataset uses 1.8120574951171875 MB

In [8]:

```
# training data top rows
train_sample.head()
```

Out[8]:

	ip	app	device	os	channel	click_time	is_attributed
0	22004	12	1	13	497	2017-11-07 09:30:38	0
1	40024	25	1	17	259	2017-11-07 13:40:27	0
2	35888	12	1	19	212	2017-11-07 18:05:24	0
3	29048	13	1	13	477	2017-11-07 04:58:08	0
4	2877	12	1	1	178	2017-11-09 09:00:09	0

## Exploring the Data - Univariate Analysis

Let's now understand and explore the data. Let's start with understanding the size and data types of the train\_sample data.

In [11]:

```
# Look at non-null values, number of entries etc.
# there are no missing values
train_sample.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 100000 entries, 0 to 99999
Data columns (total 7 columns):
ip           100000 non-null uint16
app          100000 non-null uint16
device       100000 non-null uint16
os           100000 non-null uint16
channel      100000 non-null uint16
click_time   100000 non-null object
is_attributed 100000 non-null uint8
dtypes: object(1), uint16(5), uint8(1)
memory usage: 1.8+ MB
```

In [15]:

```
# Basic exploratory analysis

# Number of unique values in each column
def fraction_unique(x):
    return len(train_sample[x].unique())

number_unique_vals = {x: fraction_unique(x) for x in train_sample.columns}
number_unique_vals
```

Out[15]:

```
{'app': 161,
 'channel': 161,
 'click_time': 80350,
 'device': 100,
 'ip': 28470,
 'is_attributed': 2,
 'os': 130}
```

In [23]:

```
# All columns apart from click time are originally int type,
# though note that they are all actually categorical
train_sample.dtypes
```

Out[23]:

```
ip          uint16
app         uint16
device      uint16
os          uint16
channel     uint16
click_time   object
is_attributed  uint8
dtype: object
```

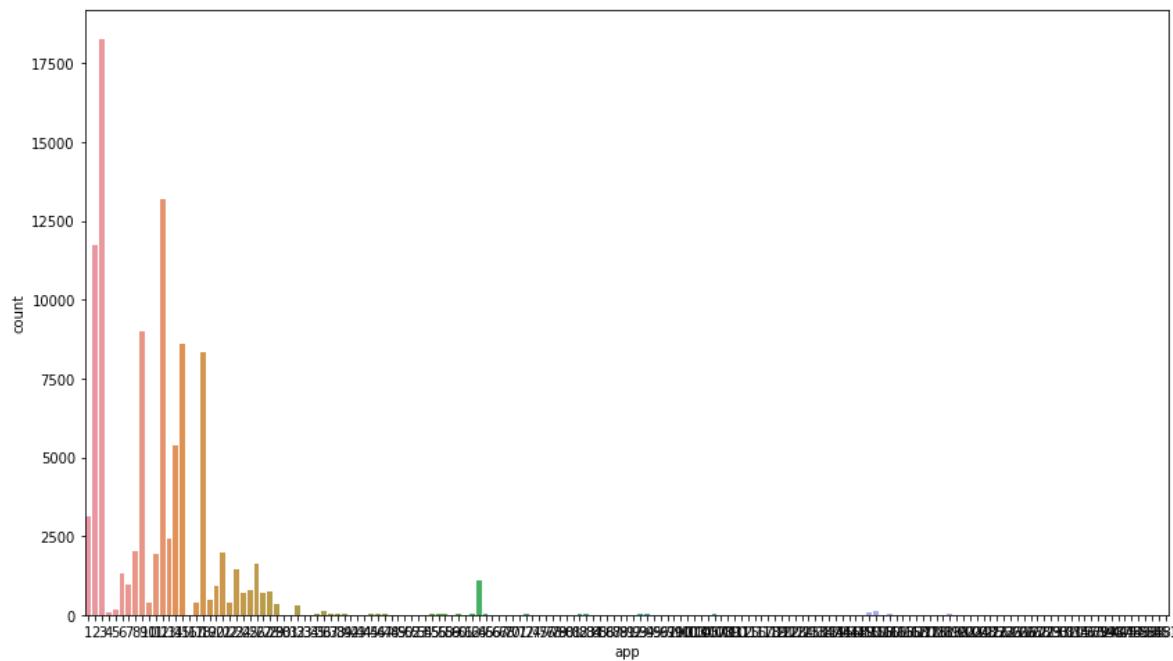
There are certain 'apps' which have quite high number of instances/rows (each row is a click). The plot below shows this.

In [24]:

```
# # distribution of 'app'  
# # some 'apps' have a disproportionately high number of clicks (>15k), and some are very r  
plt.figure(figsize=(14, 8))  
sns.countplot(x="app", data=train_sample)
```

Out[24]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x10beb5518>
```

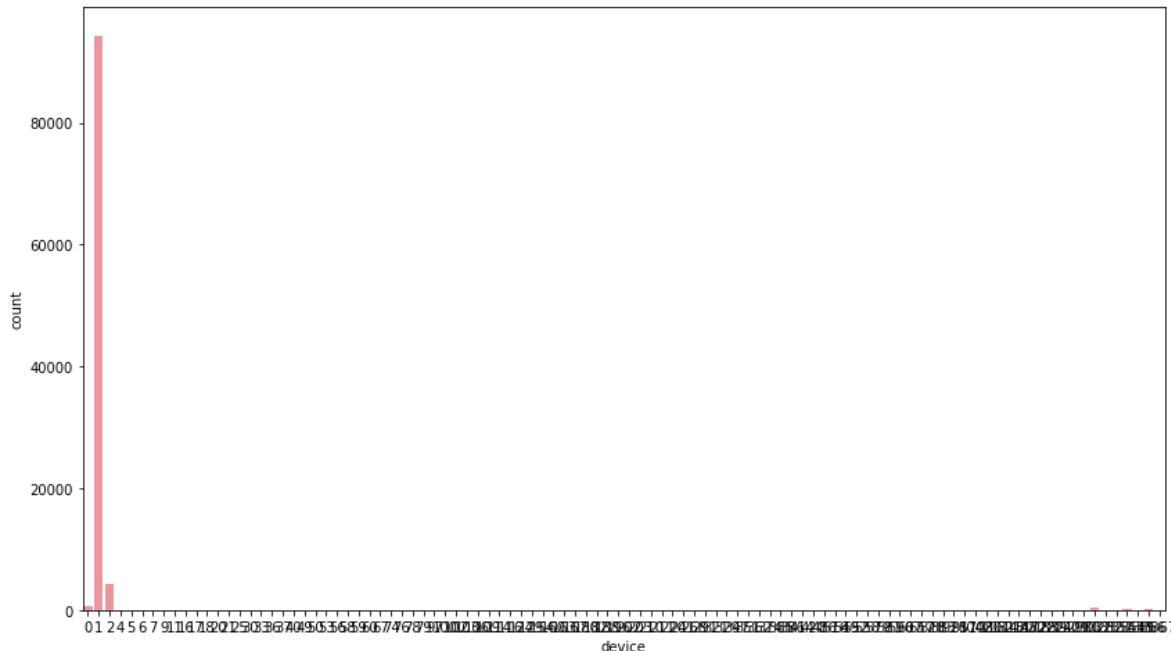


In [25]:

```
# # distribution of 'device'  
# # this is expected because a few popular devices are used heavily  
plt.figure(figsize=(14, 8))  
sns.countplot(x="device", data=train_sample)
```

Out[25]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x10bfd9978>
```

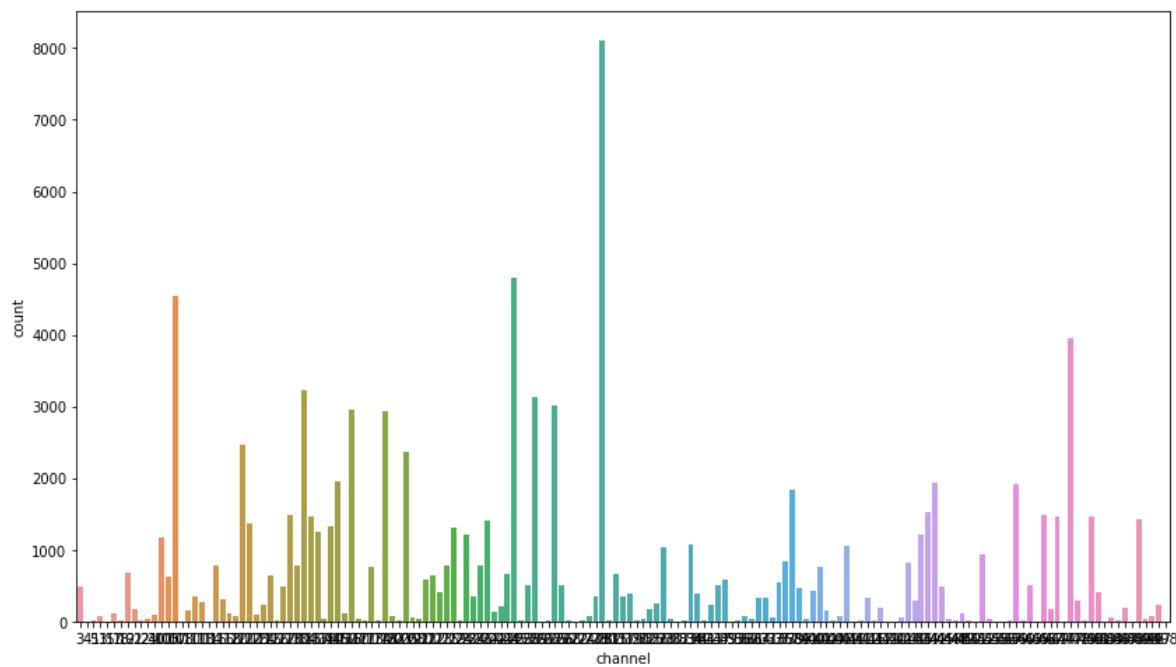


In [26]:

```
# # channel: various channels get clicks in comparable quantities
plt.figure(figsize=(14, 8))
sns.countplot(x="channel", data=train_sample)
```

Out[26]:

```
<matplotlib.axes._subplots.AxesSubplot at 0x10c523940>
```

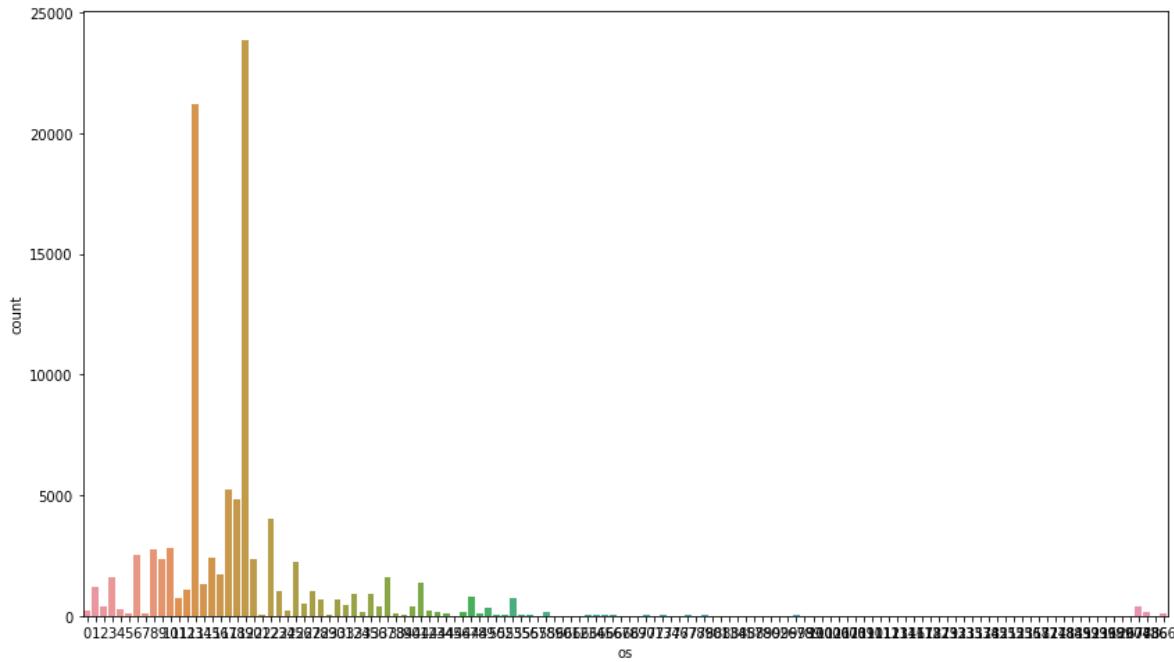


In [27]:

```
# # os: there are a couple commos OSes (android and ios?), though some are rare and can ind
plt.figure(figsize=(14, 8))
sns.countplot(x="os", data=train_sample)
```

Out[27]:

&lt;matplotlib.axes.\_subplots.AxesSubplot at 0x10ba40ef0&gt;



Let's now look at the distribution of the target variable 'is\_attributed'.

In [28]:

```
# # target variable distribution
100*(train_sample['is_attributed'].astype('object').value_counts()/len(train_sample.index))
```

Out[28]:

0	99.773
1	0.227
Name: is_attributed, dtype: float64	

Only **about 0.2% of clicks are 'fraudulent'**, which is expected in a fraud detection problem. Such high class imbalance is probably going to be the toughest challenge of this problem.

## Exploring the Data - Segmented Univariate Analysis

Let's now look at how the target variable varies with the various predictors.

In [35]:

```
# plot the average of 'is_attributed', or 'download rate'
# with app (clearly this is non-readable)
app_target = train_sample.groupby('app').is_attributed.agg(['mean', 'count'])
app_target
```

Out[35]:

	mean	count
<b>app</b>		

<b>1</b>	0.000000	3135
<b>2</b>	0.000000	11737
<b>3</b>	0.000219	18279
<b>4</b>	0.000000	58
<b>5</b>	0.074468	188
<b>6</b>	0.000000	1303
<b>7</b>	0.000000	981
<b>8</b>	0.001996	2004
<b>9</b>	0.000890	8992
<b>10</b>	0.046392	388

This is clearly non-readable, so let's first get rid of all the apps that are very rare (say which comprise of less than 20% clicks) and plot the rest.

In [63]:

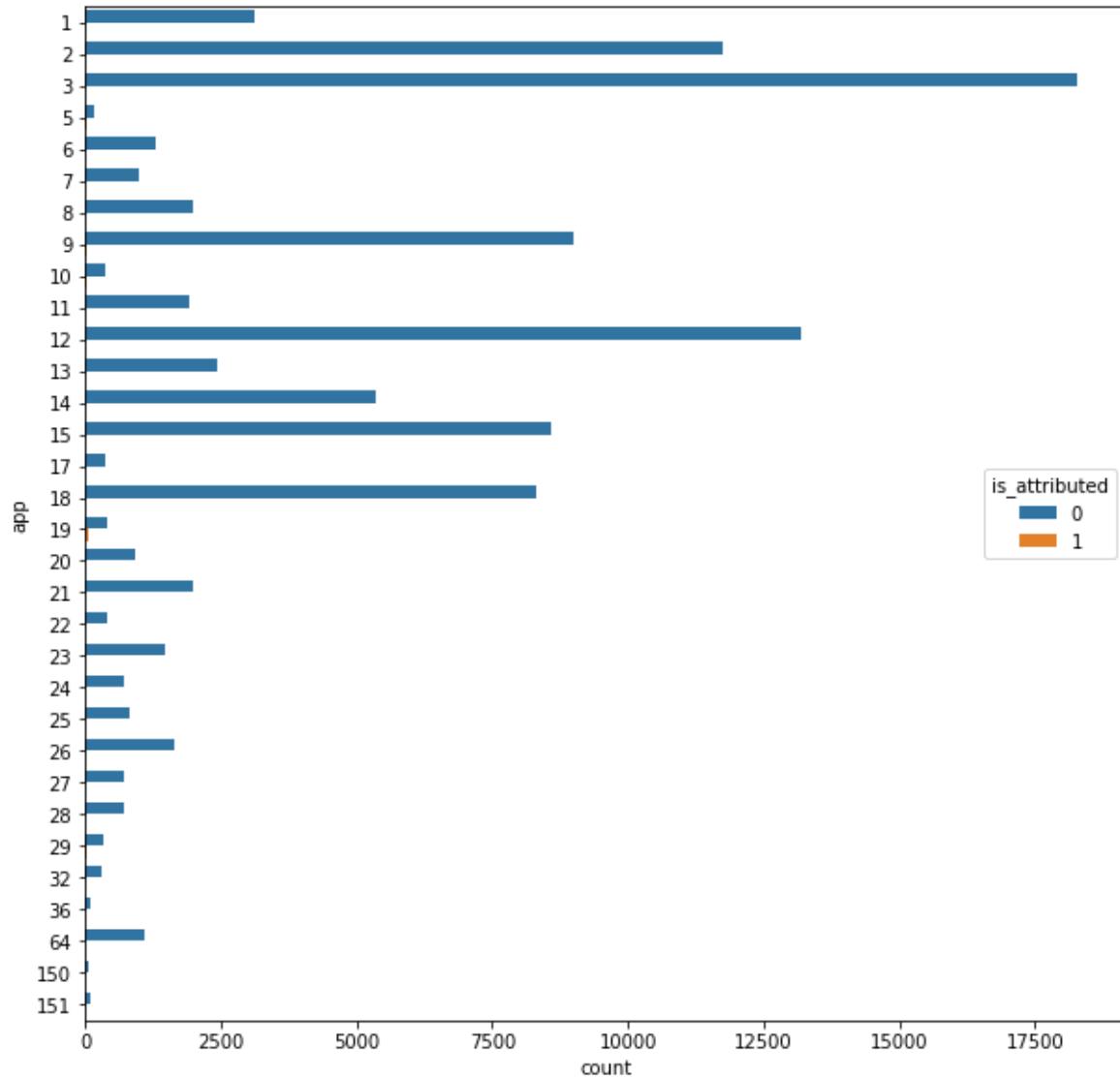
```
frequent_apps = train_sample.groupby('app').size().reset_index(name='count')
frequent_apps = frequent_apps[frequent_apps['count'] > frequent_apps['count'].quantile(0.80)]
frequent_apps = frequent_apps.merge(train_sample, on='app', how='inner')
frequent_apps.head()
```

Out[63]:

app	count	ip	device	os	channel	is_attributed	day_of_week	day_of_year	month	h
<b>0</b>	1	3135	17059	1	17	135	0	3	313	11
<b>1</b>	1	3135	52432	1	13	115	0	1	311	11
<b>2</b>	1	3135	23706	1	27	124	0	1	311	11
<b>3</b>	1	3135	58458	1	19	101	0	3	313	11
<b>4</b>	1	3135	34067	1	15	134	0	1	311	11

In [64]:

```
plt.figure(figsize=(10,10))
sns.countplot(y="app", hue="is_attributed", data=frequent_apps);
```



You can do lots of other interesting analysis with the existing features. For now, let's create some new features which will probably improve the model.

## Feature Engineering

Let's now derive some new features from the existing ones. There are a number of features one can extract from `click_time` itself, and by grouping combinations of IP with other features.

### Datetime Based Features

In [45]:

```
# Creating datetime variables
# takes in a df, adds date/time based columns to it, and returns the modified df
def timeFeatures(df):
    # Derive new features using the click_time column
    df['datetime'] = pd.to_datetime(df['click_time'])
    df['day_of_week'] = df['datetime'].dt.dayofweek
    df["day_of_year"] = df["datetime"].dt.dayofyear
    df["month"] = df["datetime"].dt.month
    df["hour"] = df["datetime"].dt.hour
    return df
```

In [46]:

```
# creating new datetime variables and dropping the old ones
train_sample = timeFeatures(train_sample)
train_sample.drop(['click_time', 'datetime'], axis=1, inplace=True)
train_sample.head()
```

Out[46]:

	ip	app	device	os	channel	is_attributed	day_of_week	day_of_year	month	hour
0	22004	12	1	13	497	0	1	311	11	9
1	40024	25	1	17	259	0	1	311	11	13
2	35888	12	1	19	212	0	1	311	11	18
3	29048	13	1	13	477	0	1	311	11	4
4	2877	12	1	1	178	0	3	313	11	9

In [65]:

```
# datatypes
# note that by default the new datetime variables are int64
train_sample.dtypes
```

Out[65]:

ip	uint16
app	uint16
device	uint16
os	uint16
channel	uint16
is_attributed	uint8
day_of_week	int64
day_of_year	int64
month	int64
hour	int64
dtype:	object

In [66]:

```
# memory used by training data
print('Training dataset uses {0} MB'.format(train_sample.memory_usage().sum()/1024**2))
```

Training dataset uses 4.1008758544921875 MB

In [67]:

```
# lets convert the variables back to Lower dtype again
int_vars = ['app', 'device', 'os', 'channel', 'day_of_week','day_of_year', 'month', 'hour']
train_sample[int_vars] = train_sample[int_vars].astype('uint16')
```

In [68]:

```
train_sample.dtypes
```

Out[68]:

```
ip          uint16
app         uint16
device      uint16
os          uint16
channel     uint16
is_attributed  uint8
day_of_week   uint16
day_of_year    uint16
month        uint16
hour          uint16
dtype: object
```

In [69]:

```
# space used by training data
print('Training dataset uses {0} MB'.format(train_sample.memory_usage().sum()/1024**2))
```

Training dataset uses 1.8120574951171875 MB

## IP Grouping Based Features

Let's now create some important features by grouping IP addresses with features such as os, channel, hour, day etc. Also, count of each IP address will also be a feature.

Note that though we are deriving new features by grouping IP addresses, using IP address itself as a features is not a good idea. This is because (in the test data) if a new IP address is seen, the model will see a new 'category' and will not be able to make predictions (IP is a categorical variable, it has just been encoded with numbers).

In [71]:

```
# number of clicks by count of IP address
# note that we are explicitly asking pandas to re-encode the aggregated features
# as 'int16' to save memory
ip_count = train_sample.groupby('ip').size().reset_index(name='ip_count').astype('int16')
ip_count.head()
```

Out[71]:

	ip	ip_count
0	8	1
1	9	1
2	10	3
3	14	1
4	16	6

We can now merge this dataframe with the original training df. Similarly, we can create combinations of various features such as ip\_day\_hour (count of ip-day-hour combinations), ip\_hour\_channel, ip\_hour\_app, etc.

The following function takes in a dataframe and creates these features.

In [73]:

```
# creates groupings of IP addresses with other features and appends the new features to the df
def grouped_features(df):
    # ip_count
    ip_count = df.groupby('ip').size().reset_index(name='ip_count').astype('uint16')
    ip_day_hour = df.groupby(['ip', 'day_of_week', 'hour']).size().reset_index(name='ip_day_hour')
    ip_hour_channel = df[['ip', 'hour', 'channel']].groupby(['ip', 'hour', 'channel']).size()
    ip_hour_os = df.groupby(['ip', 'hour', 'os']).channel.count().reset_index(name='ip_hour_os')
    ip_hour_app = df.groupby(['ip', 'hour', 'app']).channel.count().reset_index(name='ip_hour_app')
    ip_hour_device = df.groupby(['ip', 'hour', 'device']).channel.count().reset_index(name='ip_hour_device')

    # merge the new aggregated features with the df
    df = pd.merge(df, ip_count, on='ip', how='left')
    del ip_count
    df = pd.merge(df, ip_day_hour, on=['ip', 'day_of_week', 'hour'], how='left')
    del ip_day_hour
    df = pd.merge(df, ip_hour_channel, on=['ip', 'hour', 'channel'], how='left')
    del ip_hour_channel
    df = pd.merge(df, ip_hour_os, on=['ip', 'hour', 'os'], how='left')
    del ip_hour_os
    df = pd.merge(df, ip_hour_app, on=['ip', 'hour', 'app'], how='left')
    del ip_hour_app
    df = pd.merge(df, ip_hour_device, on=['ip', 'hour', 'device'], how='left')
    del ip_hour_device

    return df
```

In [75]:

```
train_sample = grouped_features(train_sample)
```

In [76]:

```
train_sample.head()
```

Out[76]:

	ip	app	device	os	channel	is_attributed	day_of_week	day_of_year	month	hour	ip_
0	22004	12	1	13	497	0	1	311	11	9	
1	40024	25	1	17	259	0	1	311	11	13	
2	35888	12	1	19	212	0	1	311	11	18	
3	29048	13	1	13	477	0	1	311	11	4	
4	2877	12	1	1	178	0	3	313	11	9	



In [77]:

```
print('Training dataset uses {0} MB'.format(train_sample.memory_usage().sum()/1024**2))
```

Training dataset uses 3.719329833984375 MB

In [79]:

```
# garbage collect (unused) object
gc.collect()
```

Out[79]:

17431

## Modelling

Let's now build models to predict the variable `is_attributed` (downloaded). We'll try the several variants of boosting (adaboost, gradient boosting and XGBoost), tune the hyperparameters in each model and choose the one which gives the best performance.

In the original Kaggle competition, the metric for model evaluation is **area under the ROC curve**.

In [83]:

```
# create x and y train
X = train_sample.drop('is_attributed', axis=1)
y = train_sample[['is_attributed']]

# split data into train and test/validation sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20, random_state=101)
print(X_train.shape)
print(y_train.shape)
print(X_test.shape)
print(y_test.shape)
```

```
(80000, 15)
(80000, 1)
(20000, 15)
(20000, 1)
```

In [84]:

```
# check the average download rates in train and test data, should be comparable
print(y_train.mean())
print(y_test.mean())
```

```
is_attributed    0.002275
dtype: float64
is_attributed    0.00225
dtype: float64
```

## AdaBoost

In [105]:

```
# adaboost classifier with max 600 decision trees of depth=2
# Learning_rate/shrinkage=1.5

# base estimator
tree = DecisionTreeClassifier(max_depth=2)

# adaboost with the tree as base estimator
adaboost_model_1 = AdaBoostClassifier(
    base_estimator=tree,
    n_estimators=600,
    learning_rate=1.5,
    algorithm="SAMME")
```

In [106]:

```
# fit
adaboost_model_1.fit(X_train, y_train)
```

Out[106]:

```
AdaBoostClassifier(algorithm='SAMME',
                   base_estimator=DecisionTreeClassifier(class_weight=None, criterion
='gini', max_depth=2,
                                               max_features=None, 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, presort=False, random_state=None,
                                               splitter='best'),
                   learning_rate=1.5, n_estimators=600, random_state=None)
```

In [107]:

```
# predictions
# the second column represents the probability of a click resulting in a download
predictions = adaboost_model_1.predict_proba(X_test)
predictions[:10]
```

Out[107]:

```
array([[ 0.5259697 ,  0.4740303 ],
       [ 0.52720083,  0.47279917],
       [ 0.533081  ,  0.466919  ],
       [ 0.52194781,  0.47805219],
       [ 0.51032691,  0.48967309],
       [ 0.52721323,  0.47278677],
       [ 0.5183883 ,  0.4816117 ],
       [ 0.52170927,  0.47829073],
       [ 0.52412251,  0.47587749],
       [ 0.51552875,  0.48447125]])
```

In [108]:

```
# metrics: AUC
metrics.roc_auc_score(y_test, predictions[:,1])
```

Out[108]:

```
0.92838553411843305
```

## AdaBoost - Hyperparameter Tuning

Let's now tune the hyperparameters of the AdaBoost classifier. In this case, we have two types of hyperparameters - those of the component trees (max\_depth etc.) and those of the ensemble (n\_estimators, learning\_rate etc.).

We can tune both using the following technique - the keys of the form `base_estimator_parameter_name` belong to the trees (base estimator), and the rest belong to the ensemble.

In [171]:

```
# parameter grid
param_grid = {"base_estimator__max_depth": [2, 5],
              "n_estimators": [200, 400, 600]
             }
```

In [163]:

```
# base estimator
tree = DecisionTreeClassifier()

# adaboost with the tree as base estimator
# Learning rate is arbitrarily set to 0.6, we'll discuss learning_rate below
ABC = AdaBoostClassifier(
    base_estimator=tree,
    learning_rate=0.6,
    algorithm="SAMME")
```

In [164]:

```
# run grid search
folds = 3
grid_search_ABC = GridSearchCV(ABC,
                               cv = folds,
                               param_grid=param_grid,
                               scoring = 'roc_auc',
                               return_train_score=True,
                               verbose = 1)
```

In [165]:

```
# fit
grid_search_ABC.fit(X_train, y_train)
```

Fitting 3 folds for each of 6 candidates, totalling 18 fits

[Parallel(n\_jobs=1)]: Done 18 out of 18 | elapsed: 10.1min finished

Out[165]:

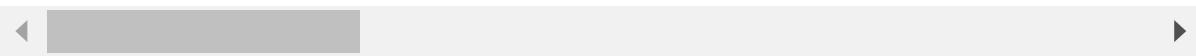
```
GridSearchCV(cv=3, error_score='raise',
            estimator=AdaBoostClassifier(algorithm='SAMME',
                                         base_estimator=DecisionTreeClassifier(class_weight=None, criterion
                                         ='gini', max_depth=None,
                                         max_features=None, 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, presort=False, random_state=None,
                                         splitter='best'),
                                         learning_rate=0.6, n_estimators=50, random_state=None),
            fit_params=None, iid=True, n_jobs=1,
            param_grid={'n_estimators': [200, 400, 600], 'base_estimator__max_depth': [2, 5]},
            pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
            scoring='roc_auc', verbose=1)
```

In [166]:

```
# cv results
cv_results = pd.DataFrame(grid_search_ABC.cv_results_)
cv_results
```

Out[166]:

	mean_fit_time	mean_score_time	mean_test_score	mean_train_score	param_base_estimator_
0	9.376183	0.209405	0.952831	0.995954	
1	19.704252	0.450558	0.950575	0.997556	
2	30.060021	0.651644	0.949670	0.998278	
3	22.058344	0.310703	0.927757	1.000000	
4	44.099881	0.596813	0.925812	1.000000	
5	67.404276	0.879526	0.916619	1.000000	

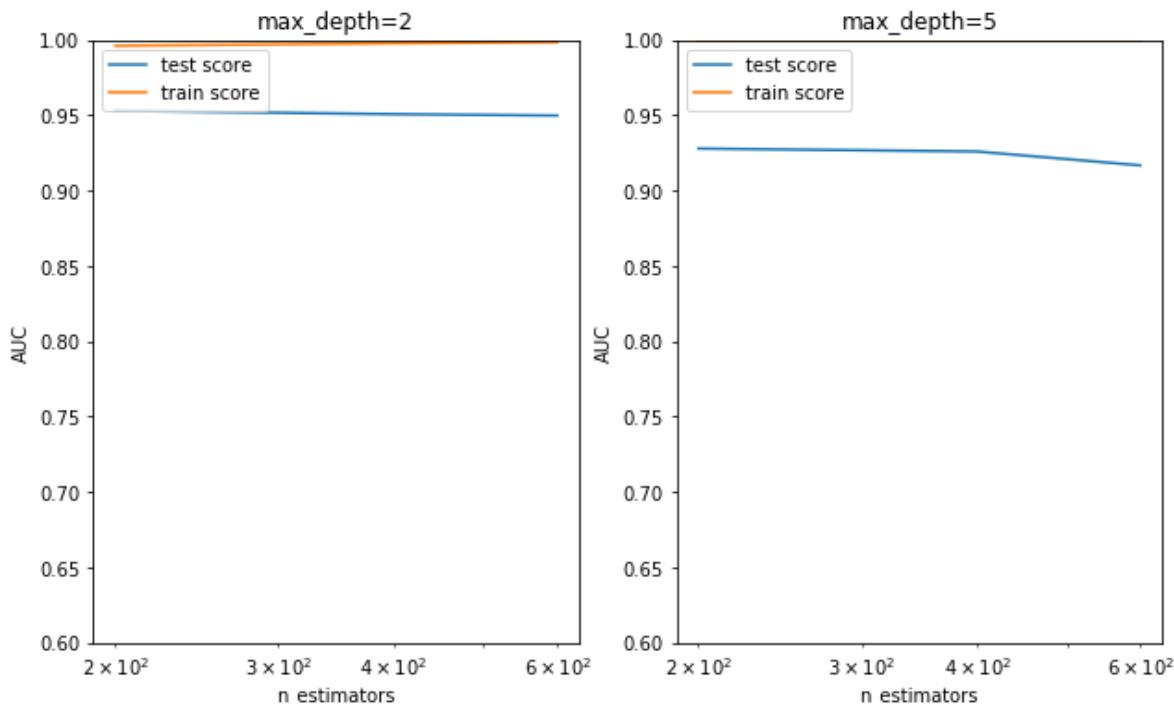


In [170]:

```
# plotting AUC with hyperparameter combinations

plt.figure(figsize=(16,6))
for n, depth in enumerate(param_grid['base_estimator__max_depth']):
    # subplot 1/n
    plt.subplot(1,3, n+1)
    depth_df = cv_results[cv_results['param_base_estimator__max_depth']==depth]

    plt.plot(depth_df["param_n_estimators"], depth_df["mean_test_score"])
    plt.plot(depth_df["param_n_estimators"], depth_df["mean_train_score"])
    plt.xlabel('n_estimators')
    plt.ylabel('AUC')
    plt.title("max_depth={0}".format(depth))
    plt.ylim([0.60, 1])
    plt.legend(['test score', 'train score'], loc='upper left')
    plt.xscale('log')
```



The results above show that:

- The ensemble with `max_depth=5` is clearly overfitting (training auc is almost 1, while the test score is much lower)
- At `max_depth=2`, the model performs slightly better (approx 95% AUC) with a higher test score

Thus, we should go ahead with `max_depth=2` and `n_estimators=200`.

Note that we haven't experimented with many other important hyperparameters till now, such as `learning_rate`, `subsample` etc., and the results might be considerably improved by tuning them. We'll next experiment with these hyperparameters.

In [183]:

```
# model performance on test data with chosen hyperparameters

# base estimator
tree = DecisionTreeClassifier(max_depth=2)

# adaboost with the tree as base estimator
# Learning rate is arbitrarily set, we'll discuss Learning_rate below
ABC = AdaBoostClassifier(
    base_estimator=tree,
    learning_rate=0.6,
    n_estimators=200,
    algorithm="SAMME")

ABC.fit(X_train, y_train)
```

Out[183]:

```
AdaBoostClassifier(algorithm='SAMME',
                   base_estimator=DecisionTreeClassifier(class_weight=None, criterion
='gini', max_depth=2,
                                               max_features=None, 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, presort=False, random_state=None,
                                               splitter='best'),
                   learning_rate=0.6, n_estimators=200, random_state=None)
```

In [184]:

```
# predict on test data
predictions = ABC.predict_proba(X_test)
predictions[:10]
```

Out[184]:

```
array([[ 0.5880972 ,  0.4119028 ],
       [ 0.58960261,  0.41039739],
       [ 0.60708804,  0.39291196],
       [ 0.57134614,  0.42865386],
       [ 0.55591021,  0.44408979],
       [ 0.58624788,  0.41375212],
       [ 0.56320517,  0.43679483],
       [ 0.58981139,  0.41018861],
       [ 0.59090843,  0.40909157],
       [ 0.56433022,  0.43566978]])
```

In [185]:

```
# roc auc
metrics.roc_auc_score(y_test, predictions[:, 1])
```

Out[185]:

0.94789331551546541

## Gradient Boosting Classifier

Let's now try the gradient boosting classifier. We'll experiment with two main hyperparameters now - `learning_rate` (shrinkage) and `subsample`.

By adjusting the learning rate to less than 1, we can regularize the model. A model with higher `learning_rate` learns fast, but is prone to overfitting; one with a lower learning rate learns slowly, but avoids overfitting.

Also, there's a trade-off between `learning_rate` and `n_estimators` - the higher the learning rate, the lesser trees the model needs (and thus we usually tune only one of them).

Also, by subsampling (setting `subsample` to less than 1), we can have the individual models built on random subsamples of size `subsample`. That way, each tree will be trained on different subsets and reduce the model's variance.

In [186]:

```
# parameter grid
param_grid = {"learning_rate": [0.2, 0.6, 0.9],
              "subsample": [0.3, 0.6, 0.9]
            }
```

In [187]:

```
# adaboost with the tree as base estimator
GBC = GradientBoostingClassifier(max_depth=2, n_estimators=200)
```

In [155]:

```
# run grid search
folds = 3
grid_search_GBC = GridSearchCV(GBC,
                                cv = folds,
                                param_grid=param_grid,
                                scoring = 'roc_auc',
                                return_train_score=True,
                                verbose = 1)

grid_search_GBC.fit(X_train, y_train)
```

Fitting 3 folds for each of 9 candidates, totalling 27 fits

[Parallel(n\_jobs=1)]: Done 27 out of 27 | elapsed: 6.8min finished

Out[155]:

```
GridSearchCV(cv=3, error_score='raise',
             estimator=GradientBoostingClassifier(criterion='friedman_mse', init=None,
             learning_rate=0.1, loss='deviance', max_depth=400,
             max_features=None, 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,
             presort='auto', random_state=None, subsample=1.0, verbose=0,
             warm_start=False),
             fit_params=None, iid=True, n_jobs=1,
             param_grid={'learning_rate': [0.2, 0.6, 0.9], 'subsample': [0.3, 0.6,
             0.9]},
             pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
             scoring='roc_auc', verbose=1)
```

In [199]:

```
cv_results = pd.DataFrame(grid_search_GBC.cv_results_)
cv_results.head()
```

Out[199]:

	mean_fit_time	mean_score_time	mean_test_score	mean_train_score	param_learning_rate	param_subsample
0	16.663277	0.110181	0.928349	0.997548	0.2	
1	19.186795	0.112623	0.746107	0.999029	0.2	
2	9.152588	0.058281	0.567046	0.999806	0.2	
3	16.168680	0.110494	0.897310	0.997573	0.6	

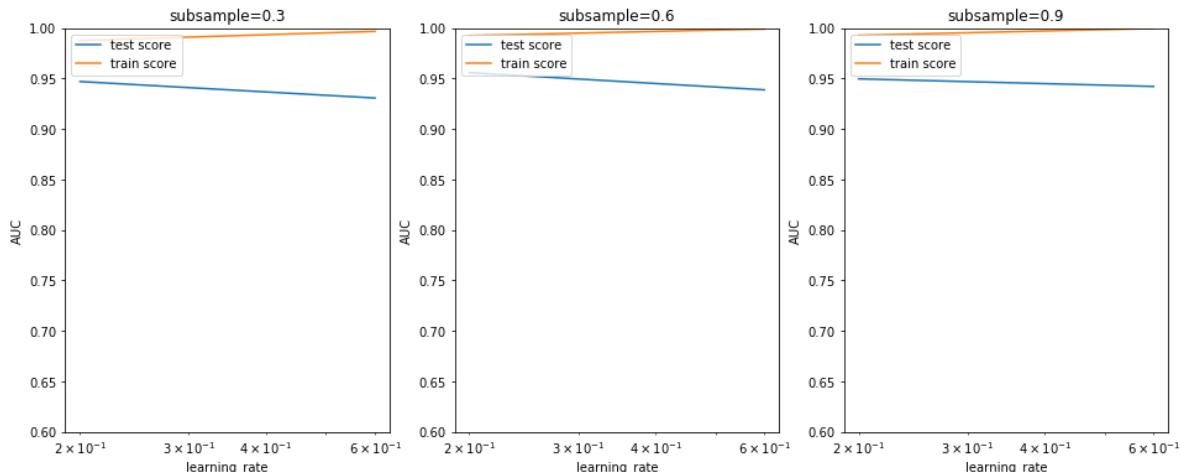
In [207]:

```
# # plotting
plt.figure(figsize=(16,6))

for n, subsample in enumerate(param_grid['subsample']):

    # subplot 1/n
    plt.subplot(1,len(param_grid['subsample']), n+1)
    df = cv_results[cv_results['param_subsample']==subsample]

    plt.plot(df["param_learning_rate"], df["mean_test_score"])
    plt.plot(df["param_learning_rate"], df["mean_train_score"])
    plt.xlabel('learning_rate')
    plt.ylabel('AUC')
    plt.title("subsample={0}".format(subsample))
    plt.ylim([0.60, 1])
    plt.legend(['test score', 'train score'], loc='upper left')
    plt.xscale('log')
```



It is clear from the plot above that the model with a lower subsample ratio performs better, while those with higher subsamples tend to overfit.

Also, a lower learning rate results in less overfitting.

## XGBoost

Let's finally try XGBoost. The hyperparameters are the same, some important ones being `subsample` , `learning_rate` , `max_depth` etc.

In [188]:

```
# fit model on training data with default hyperparameters
model = XGBClassifier()
model.fit(X_train, y_train)
```

Out[188]:

```
XGBClassifier(base_score=0.5, booster='gbtree', colsample_bylevel=1,
              colsample_bytree=1, gamma=0, learning_rate=0.1, max_delta_step=0,
              max_depth=3, min_child_weight=1, missing=None, n_estimators=100,
              n_jobs=1, nthread=None, objective='binary:logistic', random_state=0,
              reg_alpha=0, reg_lambda=1, scale_pos_weight=1, seed=None,
              silent=True, subsample=1)
```

In [189]:

```
# make predictions for test data
# use predict_proba since we need probabilities to compute auc
y_pred = model.predict_proba(X_test)
y_pred[:10]
```

Out[189]:

```
array([[ 9.99876201e-01,  1.23777572e-04],
       [ 9.99802351e-01,  1.97641290e-04],
       [ 9.99812186e-01,  1.87795449e-04],
       [ 9.99353409e-01,  6.46599103e-04],
       [ 9.98394549e-01,  1.60545984e-03],
       [ 9.99828875e-01,  1.71130727e-04],
       [ 9.99547005e-01,  4.52976237e-04],
       [ 9.99449134e-01,  5.50867291e-04],
       [ 9.99769509e-01,  2.30486505e-04],
       [ 9.96964693e-01,  3.03530321e-03]], dtype=float32)
```

In [190]:

```
# evaluate predictions
roc = metrics.roc_auc_score(y_test, y_pred[:, 1])
print("AUC: %.2f%%" % (roc * 100.0))
```

AUC: 94.85%

The roc\_auc in this case is about 0.95% with default hyperparameters. Let's try changing the hyperparameters - an exhaustive list of XGBoost hyperparameters is here: [\(http://xgboost.readthedocs.io/en/latest/parameter.html\)](http://xgboost.readthedocs.io/en/latest/parameter.html)

Let's now try tuning the hyperparameters using k-fold CV. We'll then use grid search CV to find the optimal values of hyperparameters.

In [197]:

```
# hyperparameter tuning with XGBoost

# creating a KFold object
folds = 3

# specify range of hyperparameters
param_grid = {'learning_rate': [0.2, 0.6],
              'subsample': [0.3, 0.6, 0.9]}

# specify model
xgb_model = XGBClassifier(max_depth=2, n_estimators=200)

# set up GridSearchCV()
model_cv = GridSearchCV(estimator = xgb_model,
                        param_grid = param_grid,
                        scoring= 'roc_auc',
                        cv = folds,
                        verbose = 1,
                        return_train_score=True)
```

In [198]:

```
# fit the model
model_cv.fit(X_train, y_train)
```

Fitting 3 folds for each of 6 candidates, totalling 18 fits

[Parallel(n\_jobs=1)]: Done 18 out of 18 | elapsed: 1.3min finished

Out[198]:

```
GridSearchCV(cv=3, error_score='raise',
            estimator=XGBClassifier(base_score=0.5, booster='gbtree', colsample_b
ylevel=1,
            colsample_bytree=1, gamma=0, learning_rate=0.1, max_delta_step=0,
            max_depth=2, min_child_weight=1, missing=None, n_estimators=200,
            n_jobs=1, nthread=None, objective='binary:logistic', random_state=0,
            reg_alpha=0, reg_lambda=1, scale_pos_weight=1, seed=None,
            silent=True, subsample=1),
            fit_params=None, iid=True, n_jobs=1,
            param_grid={'learning_rate': [0.2, 0.6], 'subsample': [0.3, 0.6, 0.
9]}, pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
            scoring='roc_auc', verbose=1)
```

In [202]:

```
# cv results
cv_results = pd.DataFrame(model_cv.cv_results_)
cv_results
```

Out[202]:

	mean_fit_time	mean_score_time	mean_test_score	mean_train_score	param_learning_rate	param_subsample
0	3.741100	0.152881	0.946876	0.987553	0.2	
1	4.502307	0.145803	0.955664	0.992432	0.2	
2	3.939432	0.142248	0.949553	0.992693	0.2	
3	3.833046	0.139765	0.930576	0.996570	0.6	

In [ ]:

```
# convert parameters to int for plotting on x-axis
cv_results['param_learning_rate'] = cv_results['param_learning_rate'].astype('float')
cv_results['param_max_depth'] = cv_results['param_max_depth'].astype('float')
cv_results.head()
```

In [203]:

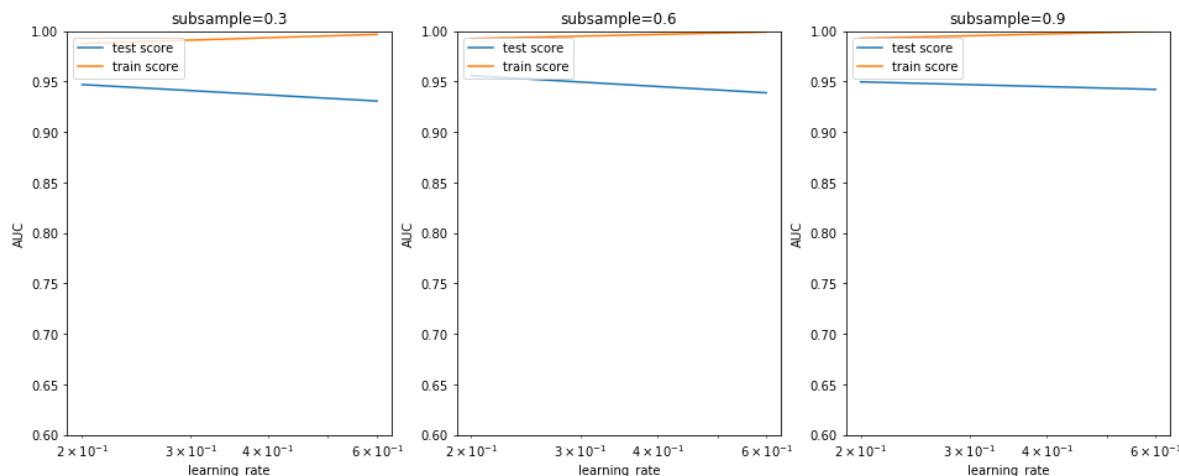
```
# # plotting
plt.figure(figsize=(16,6))

param_grid = {'learning_rate': [0.2, 0.6],
              'subsample': [0.3, 0.6, 0.9]}

for n, subsample in enumerate(param_grid['subsample']):

    # subplot 1/n
    plt.subplot(1,len(param_grid['subsample']), n+1)
    df = cv_results[cv_results['param_subsample']==subsample]

    plt.plot(df["param_learning_rate"], df["mean_test_score"])
    plt.plot(df["param_learning_rate"], df["mean_train_score"])
    plt.xlabel('learning_rate')
    plt.ylabel('AUC')
    plt.title("subsample={0}".format(subsample))
    plt.ylim([0.60, 1])
    plt.legend(['test score', 'train score'], loc='upper left')
    plt.xscale('log')
```



The results show that a subsample size of 0.6 and learning\_rate of about 0.2 seems optimal. Also, XGBoost has resulted in the highest ROC AUC obtained (across various hyperparameters).

Let's build a final model with the chosen hyperparameters.

In [204]:

```
# chosen hyperparameters
# 'objective':'binary:logistic' outputs probability rather than Label, which we need for au
params = {'learning_rate': 0.2,
           'max_depth': 2,
           'n_estimators':200,
           'subsample':0.6,
           'objective':'binary:logistic'}

# fit model on training data
model = XGBClassifier(params = params)
model.fit(X_train, y_train)
```

Out[204]:

```
XGBClassifier(base_score=0.5, booster='gbtree', colsample_bylevel=1,
              colsample_bytree=1, gamma=0, learning_rate=0.1, max_delta_step=0,
              max_depth=3, min_child_weight=1, missing=None, n_estimators=100,
              n_jobs=1, nthread=None, objective='binary:logistic',
              params={'n_estimators': 200, 'max_depth': 2, 'learning_rate': 0.2, 's
ubsample': 0.6, 'objective': 'binary:logistic'},
              random_state=0, reg_alpha=0, reg_lambda=1, scale_pos_weight=1,
              seed=None, silent=True, subsample=1)
```

In [205]:

```
# predict
y_pred = model.predict_proba(X_test)
y_pred[:10]
```

Out[205]:

```
array([[ 9.99876201e-01,   1.23777572e-04],
       [ 9.99802351e-01,   1.97641290e-04],
       [ 9.99812186e-01,   1.87795449e-04],
       [ 9.99353409e-01,   6.46599103e-04],
       [ 9.98394549e-01,   1.60545984e-03],
       [ 9.99828875e-01,   1.71130727e-04],
       [ 9.99547005e-01,   4.52976237e-04],
       [ 9.99449134e-01,   5.50867291e-04],
       [ 9.99769509e-01,   2.30486505e-04],
       [ 9.96964693e-01,   3.03530321e-03]], dtype=float32)
```

The first column in y\_pred is the P(0), i.e. P(not fraud), and the second column is P(1/fraud).

In [206]:

```
# roc_auc
auc = sklearn.metrics.roc_auc_score(y_test, y_pred[:, 1])
auc
```

Out[206]:

```
0.94848687324257352
```

Finally, let's also look at the feature importances.

In [225]:

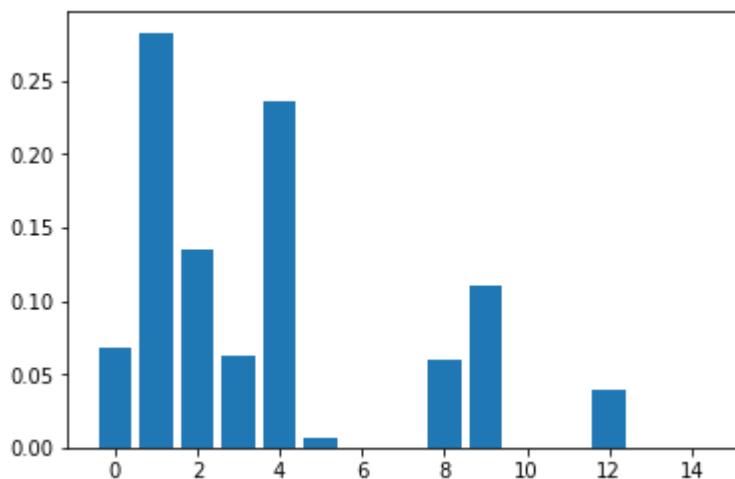
```
# feature importance
importance = dict(zip(X_train.columns, model.feature_importances_))
importance
```

Out[225]:

```
{'app': 0.28301886,
'channel': 0.23584905,
'day_of_week': 0.006289308,
'day_of_year': 0.0,
'device': 0.13522013,
'hour': 0.059748426,
'ip': 0.067610063,
'ip_count': 0.11006289,
'ip_day_hour': 0.0,
'ip_hour_app': 0.0,
'ip_hour_channel': 0.0,
'ip_hour_device': 0.0,
'ip_hour_os': 0.039308175,
'month': 0.0,
'os': 0.062893085}
```

In [228]:

```
# plot
plt.bar(range(len(model.feature_importances_)), model.feature_importances_)
plt.show()
```



## Predictions on Test Data

Since this problem is hosted on Kaggle, you can choose to make predictions on the test data and submit your results. Please note the following points and recommendations if you go ahead with Kaggle:

Recommendations for training:

- We have used only a fraction of the training set (train\_sample, 100k rows), the full training data on Kaggle (train.csv) has about 180 million rows. You'll get good results only if you train the model on a significant portion of the training dataset.
- Because of the size, you'll need to use Kaggle kernels to train the model on full training data. Kaggle kernels provide powerful computation capacities on cloud (for free).

- Even on the kernel, you may need to use a portion of the training dataset (try using the last 20-30 million rows).
- Make sure you save memory by following some tricks and best practices, else you won't be able to train the model at all on a large dataset.

In [ ]:

```
# # read submission file
# sample_sub = pd.read_csv(path+'sample_submission.csv')
# sample_sub.head()
```

In [ ]:

```
# # predict probability of test data
# test_final = pd.read_csv(path+'test.csv')
# test_final.head()
```

In [ ]:

```
# # predictions on test data
# test_final = timeFeatures(test_final)
# test_final.head()
```

In [ ]:

```
# test_final.drop(['click_time', 'datetime'], axis=1, inplace=True)
```

In [ ]:

```
# test_final.head()
```

In [ ]:

```
# test_final[categorical_cols]=test_final[categorical_cols].apply(lambda x: le.fit_transform(x))
```

In [ ]:

```
# test_final.info()
```

In [ ]:

```
# # number of clicks by IP
# ip_count = test_final.groupby('ip')['channel'].count().reset_index()
# ip_count.columns = ['ip', 'count_by_ip']
# ip_count.head()
```

In [ ]:

```
# merge this with the training data
# test_final = pd.merge(test_final, ip_count, on='ip', how='left')
```

In [ ]:

```
# del ip_count
```

In [ ]:

```
# test_final.info()
```

In [ ]:

```
# # predict on test data
# y_pred_test = model.predict_proba(test_final.drop('click_id', axis=1))
# y_pred_test[:10]
```

In [ ]:

```
# # # create submission file
# sub = pd.DataFrame()
# sub['click_id'] = test_final['click_id']
# sub['is_attributed'] = y_pred_test[:, 1]
# sub.head()
```

In [ ]:

```
# sub.to_csv('kshitij_sub_03.csv', float_format='%.8f', index=False)
```

In [ ]:

```
# # model

# dtrain = xgb.DMatrix(X_train, y_train)
# del X_train, y_train
# gc.collect()

# watchlist = [(dtrain, 'train')]
# model = xgb.train(params, dtrain, 30, watchlist, maximize=True, verbose_eval=1)
```

In [ ]:

```
# del dtrain
# gc.collect()
```

In [ ]:

```
# # Plot the feature importance from xgboost
# plot_importance(model)
# plt.gcf().savefig('feature_importance_xgb.png')
```

In [ ]:

```
# # Load the test for predict
# test = pd.read_csv(path+"test.csv")
```

In [ ]:

```
# test.head()
```

In [ ]:

```
# # number of clicks by IP
# ip_count = train_sample.groupby('ip')['channel'].count().reset_index()
# ip_count.columns = ['ip', 'count_by_ip']
# ip_count.head()
```

In [ ]:

```
# test = pd.merge(test, ip_count, on='ip', how='left', sort=False)
# gc.collect()
```

In [ ]:

```
# test = timeFeatures(test)
# test.drop(['click_time', 'datetime'], axis=1, inplace=True)
# test.head()
```

In [ ]:

```
# print(test.columns)
# print(train_sample.columns)
```

In [ ]:

```
# test = test[['click_id', 'ip', 'app', 'device', 'os', 'channel', 'day_of_week',
#             'day_of_year', 'month', 'hour', 'count_by_ip']]
```

In [ ]:

```
# dtest = xgb.DMatrix(test.drop('click_id', axis=1))
```

In [ ]:

```
# # Save the predictions
# sub = pd.DataFrame()
# sub['click_id'] = test['click_id']

# sub['is_attributed'] = model.predict(dtest, ntree_limit=model.best_ntree_limit)
# sub.to_csv('xgb_sub.csv', float_format='%.8f', index=False)
```

In [ ]:

```
# sub.shape
```



# Summary

You have come a long way! Let's look at a summary of all that you have covered in the last two sessions.

In the first session, we went through the concepts of boosting and studied one of the earliest boosting algorithms, AdaBoost. We went through the process of updating the distribution of the data points by changing the probabilities attached to them and deciding the weights attached to the individual models that fit on this distribution.

In the next session, we went through Gradient Boosting and a modification of it, XGBoost. We were introduced to the intuition of gradient descent in the regression setting when we used the square loss function to close in on the residues. We developed from here on the Gradient Boosting algorithm in which each subsequent model trains on the gradients of the loss function. XGBoost follows the same procedure on trees with additional features like regularization and parallel tree learning algorithm for finding the best split.

You can download the lecture notes for this module from the link below:



Lecture Notes - Boosting



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## Supervised Learning - Boosting

In this module, you grasped the concepts of another supervised learning algorithm called Boosting. We learned some of the popular algorithms, namely **AdaBoost**, **Gradient Boosting** and a modification of Gradient Boosting, **XGBoost**.

### Boosting

Boosting was first introduced in 1997 by Freund and Schapire in the popular algorithm, AdaBoost. It was originally designed for classification problems. Since its inception, many new boosting algorithms have been developed those tackle regression problems also and have become famous as they are used in the top solutions of many Kaggle competitions.

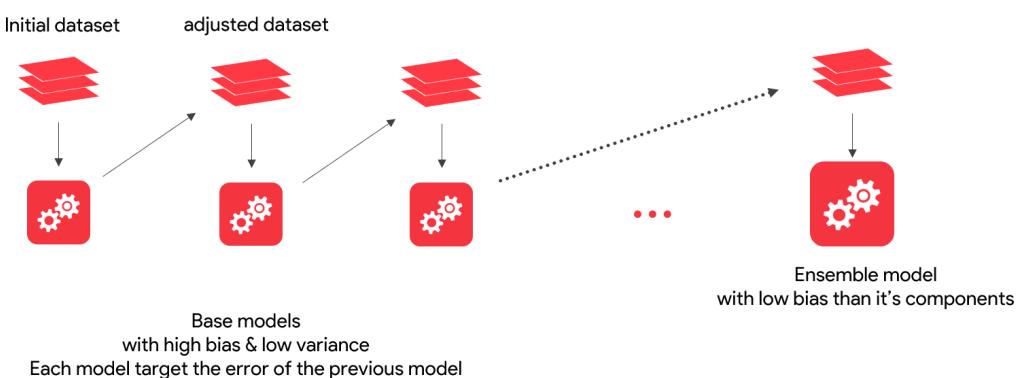
Let's start off with the basics of Boosting and move on to the boosting algorithms.

An ensemble is a collection of models which ideally should predict better than individual models. The key idea of boosting is to create an ensemble which makes high errors only on the less frequent data points.

Boosting leverages the fact that we can build a series of models specifically targeted at the data points which have been incorrectly predicted by the other models in the ensemble. If a series of models keep reducing the average error, we will have an ensemble having extremely high accuracy.

Boosting is a way of generating a strong model from a weak learning algorithm.

**A weak learning algorithm** produces a model that does marginally better than a random guess. A random guess has a 50% chance of being right. Hence, any such model created by the weak learning algorithm shall have, say 60-70% chance of being correct.



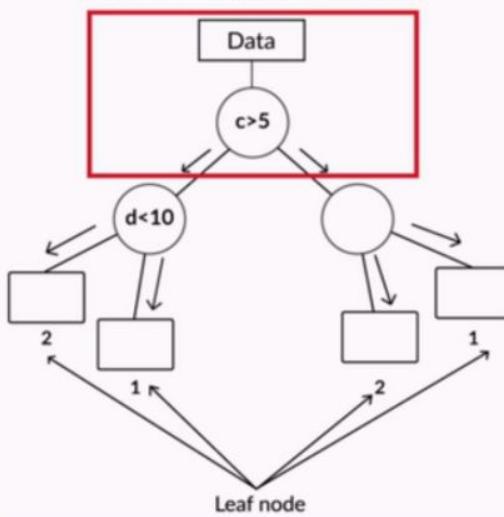
### Boosting

There are other ways we can make the decision tree a weak learner like

1. max\_depth: The maximum depth of the tree
2. min\_samples\_split: The minimum number of samples required to split an internal node
3. min\_samples\_leaf: The minimum number of samples required to be at a leaf node:
4. min\_weight\_fraction\_leaf: The minimum weighted fraction of the sum total of weights (of all the input samples) required to be at a leaf node
5. max\_leaf\_nodes: The maximum number of leaf nodes that can be generated
6. min\_impurity\_decrease: A node will be split if this split induces a decrease of the impurity greater than or equal to this value
7. min\_impurity\_split: A node will split if its impurity is above the threshold, otherwise it is a leaf

The following picture delivers an example of a weak learner. We have a learning algorithm, decision tree. By restricting the depth of the tree, we can make this decision tree a weak learner. The red box indicates only one split which is also known as a stump.

**DECISION TREE ALGORITHM**



The final objective is to create a strong model by making an ensemble of such weak models.

Here, it is important to understand the loss functions for regression and classification problems are different. Until now, we have defined the error function for a regression setting as the sum of squared difference between the actual and the predicted values while the misclassification rate for a classification problem.

### Adaboost

AdaBoost stands for Adaptive Boosting, was developed by Schapire and Freund, who later on won the 2003 Gödel Prize for their work. In this method, every subsequent model is built on a new distribution. This new distribution is created by changing the probability or weights attached with every point. Here, we explain the AdaBoost algorithm using the classification setting in which the target values are +1/-1.

At an iteration  $t$ , we have a distribution  $D_t$  of the training data  $T$ , with the data points having probability  $p_d(t)(x_i)$  on which we fit a model  $H_t$  and then use the results to create a new distribution  $D_{t+1}$ . The final model  $H$ , we build is an ensemble of all the individual models  $H_i$  with weights  $\alpha_i$ .

The AdaBoost process starts off with uniform distribution for all the points but as we move on to make additional models that add to the previous model, the distribution changes and hence, the objective function is expressed in terms of the probabilities of the different data points. The probabilities of the data points on which the next additional model is built are changed in such a way that the algorithm increases the probabilities of the points that were incorrectly classified by the current model and lowers the probabilities of the points that were correctly classified. With each new model, the distribution of the data changes.

There are essentially two steps involved in the AdaBoost algorithm:

1. Modify the current distribution to create a new distribution to generate a new model
2. Calculation of the weights given to each of the models to get the final ensemble

Here is the pseudo-code for Adaboost

1. Initialize the probabilities of the distribution as  $\frac{1}{n}$  where  $n$  is the number of data points
2. For  $t = 0$  to  $T$ , repeat the following ( $T$  is the total number of trees):
  1. Fit a tree  $h_t$  on the training data using the respective probabilities
  2. Compute  $\epsilon_t = \sum_i^n D_i[h_t(x_i) \neq y_i]$
  3. Compute  $\alpha_t = \frac{1}{2} \ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$
  4. Update  $D_{t+1}(i) = \frac{D_t(i) * e^{-\alpha_t y_i h_t(x_i)}}{z_t}$  where,  $z_t = \sum_{i=1}^n D_i * e^{-\alpha_t y_i h_t(x_i)}$
3. Final Model:  $H(x) = \text{sign}(\sum_{t=1}^T \alpha_t h_t(x))$

We can see that if the prediction is correct,  $y_i \cdot h_t(x_i) > 0$  and since  $\alpha_t > 0$  (will look about this in the next section),  $p_d(t+1)(xi) < p_d(t)(xi)$ .

Also, when the prediction is wrong,  $y_i \cdot h_t(x_i) < 0$  and since  $\alpha_t > 0$ ,  $p_d(t+1)(xi) < p_d(t)(xi)$ .

In other words, every subsequent model we build after changing the distribution has a misclassification rate, here the error,  $\epsilon_t < 0.5$ . With this in mind, we can see that the  $\alpha_t > 0$  as the error  $\epsilon_t < 0.5$ ,  $((1 - \epsilon_t) / \epsilon_t) = \text{positive}$  and the  $\ln(\text{positive}) > 0$ .

We continue this iteration until

- Low training error is achieved
- A preset number of weak learners have been added

We then make the final prediction by adding up the weighted prediction of every classifier.  $H(x) = \text{sign}(\sum_{t=1}^T \alpha_t h_t(x))$

We can realize here that as we increase the number of trees/ iterations, the error will keep on decreasing. Before you apply the AdaBoost algorithm, you should specifically remove the Outliers. Since AdaBoost tends to boost up the probabilities of misclassified points and there is a high chance that outliers will be misclassified, it will keep increasing the probability associated with the outliers and make the progress difficult. Some of the ways to remove outliers are:

- Boxplots
- Cook's distance
- Z-score

## Gradient Boosting

Gradient Boosting like AdaBoost trains many models in a gradual, additive, and sequential manner. But the major difference between the two is how they identify & handle the shortcomings of weak learners through loss functions.

To summarize here are the broader points on how does a GBM learn:

- We build the first weak learner using a sample from the training data; we will consider a decision tree as the weak learner or the base model. It may not necessarily be a stump, can grow a bigger tree but will still be weak i.e. still not be fully grown.
- Then the predictions are made on the training data using the decision tree just built.
- The gradient, in our case the residuals are computed and these residuals are the new response or target values for the next weak learner.
- A new weak learner is built with the residuals as the target values and a sample of observations from the original training data.
- Add the predictions obtained from the current weak learner to the predictions obtained from all the previous weak learners. The predictions obtained at each step are multiplied by the learning rate so that no

single model makes a huge contribution to the ensemble thereby avoiding overfitting. Essentially, with the addition of each weak learner, the model takes a very small step in the right direction.

- The next weak learner fits on the residuals obtained till now and these steps are repeated, either for a prespecified number of weak learners or if the model starts overfitting i.e. it starts to capture the niche patterns of the training data.
- GBM makes the final prediction by simply adding up the predictions from all the weak learners (multiplied by the learning rate)

Here is the pseudo-code for Gradient Boosting

At any iteration  $t$ , we repeat the following steps in the Gradient Boosting scheme of things:

1. Initialize a crude initial function  $F_0$  as  $\text{argmin} \sum_{t=1}^T L(y_i, \hat{y})$
2. For  $m = 1$  to  $M$  (where  $M$  is the number of trees)
  1. Calculate the pseudo-residuals  $r_{im} = -\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}$ , where  $F(x_i) = F_{m-1}(x_i)$ ,  
the pseudo residuals are the negative gradients for all data points
  2. Fit a base learner  $h_m(x)$  to the pseudo-residuals, i.e train it using the training set  $\sum_{i=1}^n (x_i, r_{im})$ . Here the pseudo residuals are used as the response variable.
  3. Compute the step magnitude multiplier  $\gamma_m$  (in case of tree models, compute a  $\gamma_m$  different for every leaf/prediction)  

$$\gamma_m = \text{argmin} \sum_{i=1}^n L(y_i, (F_{m-1} + \gamma * h_m(x_i)))$$
  4. Compute the next model  $F_m = F_{m-1}(x_i) + \gamma_m * h_m(x_i)$
  3. The final model is  $F_M(x)$

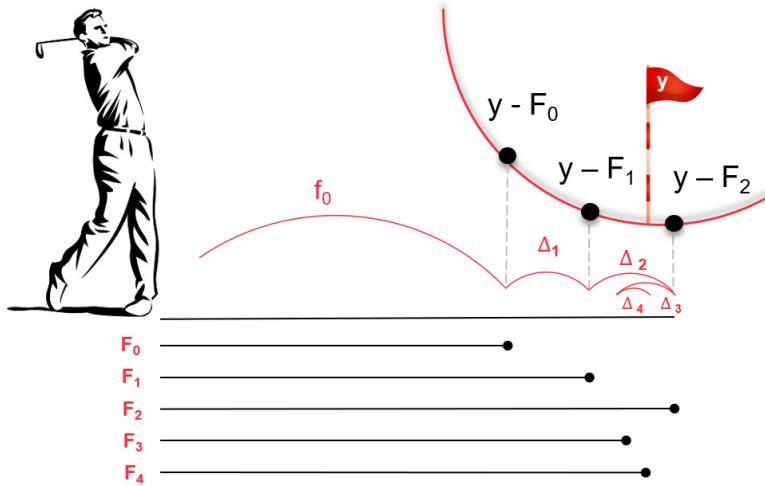
We see that the loss we get after fitting the model  $F_m$  is  $L(y_i, F_m)$ . In order to reduce this loss, we generate models  $F_m$  by adding an incremental model  $h_m(x_i)$  to  $F_{m-1}$ .

In other words, we select the  $h_m$  such that  $L(y_i, F_{m-1}) - L(y_i, F_{m-1} + h_m)$  is the maximum.

The minimization is essentially a gradient descent problem. Hence, to find an  $h_m$  which when added to  $F_{m-1}$  reduces the loss, we take a step in the direction where the Loss  $L(y_i, F_{m-1})$  reduces (with respect to  $F_{m-1}$ ).

Mathematically, we take a step of size  $\gamma$  in the direction  $-(\partial L(y_i, F(x_i))/\partial F(x_i))$ , where  $F(x_i) = F_{m-1}(x_i)$ .

We stop when we see that the gradients are very close to zero.



## Gradient Boosting

### XGBoost

**Extreme Gradient Boosting (XGBoost)** is similar to the gradient boosting framework but more efficient and advanced implementation of the Gradient Boosting algorithm.

It was first developed by Taiqi Chen and became famous in solving the Higgs Boson problem. Due to its robust accuracy, it has been widely used in machine learning competitions as well. It uses more accurate approximations to tune the model and find the best fit.

Let's have a look at some of the advantages of XGBoost:

1. **Parallel Computing:** when you run xgboost, by default, it would use all the cores of your laptop/machine enabling its capacity to do parallel computation
2. **Regularization:** The biggest advantage of xgboost is that it uses regularization and controls the overfitting and simplicity of the model which gives it better performance.
3. **Enabled Cross-Validation:** XGBoost is enabled with internal Cross Validation function
4. **Missing Values:** XGBoost is designed to handle missing values internally. The missing values are treated in such a manner that if there exists any trend in missing values, it is captured by the model.
5. **Flexibility:** XGBoost is not just limited to regression, classification, and ranking problems, it supports user-defined objective functions as well. Furthermore, it supports user-defined evaluation metrics as well.

Because of parallel processing (speed) and model performance, we can say that XGBoost is gradient boosting on steroids.

Now, let's discuss some of the frequently used parameters that are used to regularize the Tree Boosting algorithms like the Gradient Tree Boosting and the XGBoost:

$\lambda_t$ , the **learning rate**, is also known as **shrinkage**. It can be used to regularize the gradient tree boosting algorithm.  $\lambda_t$  typically varies from 0 to 1. Smaller values of  $\lambda_t$  lead to a larger value of a number of trees T (called *n\_estimators* in the Python package XGBoost). This is because, with a slower learning rate, you need a larger number of trees to reach the minima. This, in turn, leads to longer training time.

On the other hand, if  $\lambda_t$  is large, we may reach the same point with a lesser number of trees (*n\_estimators*), but there's the risk that we might actually miss the minima altogether (i.e. cross over it) because of the long stride we are taking at each iteration.

Some other ways of regularization are explicitly specifying the **number of trees T** and doing **subsampling**. Note that you shouldn't tune both  $\lambda_t$  and number of trees T together since a high  $\lambda_t$  implies a low value of T and vice-versa.

**Subsampling** is training the model in each iteration on a fraction of data (similar to how random forests build each tree). A typical value of subsampling is 0.5 while it ranges from 0 to 1. In random forests, subsampling is critical to ensure diversity among the trees, since otherwise, all the trees will start with the same training data and therefore look similar. This is not a big problem in boosting since each tree is anyway built on the residual and gets a significantly different objective function than the previous one.

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# Graded Questions

The following questions are **graded**.

< > Question 1/4 Mandatory ✓

## Gradient Boosting

Consider the following statements w.r.t Gradient Boosting and choose the correct:

1. At each iteration, we add an incremental model, which is fitted on the negative gradients of the loss function w.r.t the previous predictions.
2. We multiply  $\lambda_t$ (learning rate) with the incremental model  $h_{t+1}$  so that the new model doesn't overfit.

Only 1

Only 2

Both 1 & 2 ✓ Correct

Feedback:

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None of the above



Your answer is Correct.

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Graded Questions





# Graded Questions

The following questions are **graded**.



## Question 2/4

Mandatory



### Adaboost

In Adaboost, each model has different say/importance according to the error it has made while predicting the training data.

This is depicted in the following equation:  $\alpha = 0.5 \ln((1-\text{TOTAL ERROR})/(\text{TOTAL ERROR}))$

With respect to this, consider the following statements and choose the correct:

1. The classifier weight grows exponentially as the error approaches 0. Better classifiers are given exponentially more weight.
2. The classifier weight is 0.5 if the error rate is 0.5. This is because the classifier has only 50% accuracy.
3. The classifier weight grows exponentially negative as the error approaches 1. These types of classifiers are given a negative weight.



1 &amp; 2 only



1 &amp; 3 only

Correct

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2 & 3 only

All of the above



Your answer is Correct.

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# Graded Questions

The following questions are **graded**.



## Question 3/4

Mandatory



### General Expression for Residual

For a gradient boosting algorithm, let's say  $F_0$  is the crude model with which we start off. For a model  $F_t$  which is fitted on the training data, the prediction we get for  $x_i$  is  $F_t(x_i)$ . What is the general expression of the residuals generated once the  $F_t$  model is trained? Assume,  $y$  is the initial target variable.

$y - [F_0(x_i) + F_1(x_i) + F_2(x_i) + \dots + F_{t-2}(x_i) + F_{t-1}(x_i)]$

$y - [F_0(x_i) + F_{t-1}(x_i)]$

$y - [F_0(x_i) + F_1(x_i) + F_2(x_i) + \dots + F_{t-2}(x_i) + F_{t-1}(x_i) + F_t(x_i)]$  ✓ Correct

#### Feedback:

The residuals created by  $F_1$  is  $y - F_0(x_i) - F_1(x_i)$ , for  $F_2$  it is  $y - F_0(x_i) - F_1(x_i) - F_2(x_i)$  and so on. In general,  $F_t$  trains on the residuals generated by the model  $F_{t-1}$ . So

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# Graded Questions

The following questions are **graded**.

< > Question 4/4 Mandatory 

**XGBoost**

Which of these features are the advantages of XGBoost algorithm?

More than one option can be correct.

Parallel and distributed computing ✓ Correct

 Feedback:  
Fast learning through parallel and distributed computing enables quicker model exploration.

Optimization through first-order derivatives

Advanced regularisation ✓ Correct

 Feedback:

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# Mathematics behind XGBoost

The upcoming text discusses the maths behind the XGBoost. It is expected that you write the equations to have a better understanding.

NOTE: For a detailed understanding, please attend the live session on Saturday.

Both XGBoost and GBM follow the principle of gradient boosted trees, but XGBoost uses a more **regularised model formulation to control overfitting**, which gives it better performance, which is why it's also known as '**regularised boosting**' technique.

## The mathematics behind the XGBoost model:

Note: Here unlike the added model represented earlier by  $h_m$ , here we are representing the model by  $h_t$  at the  $t^{th}$  iteration.

In an ideal machine learning model, the objective function is a sum of Loss function “L” and regularization “ $\Omega$ ”. Loss function controls the predictive power of the algorithm and regularization controls its simplicity

**Objective Function : Training Loss(L) + Regularization( $\Omega$ )**

The algorithm we have seen in Gradient Boosting has the objective function as only the Training Loss while the XGBoost objective function constitutes of loss function evaluated

 $\tau=1$  $\tau=1$ 

Where  $h_t$  means predictions coming from the  $t^{th}$  tree.

From Gradient Boosting we have understood that the final model will be represented by:

$$F_t(x_i) = F_0(x_i) + \sum_{t=1}^T h_t(x_i) = F_{t-1}(x_i) + h_t(x_i)$$

Here  $F_t(x_i)$  is the prediction of the  $i^{th}$  instance  $x_i$  at the  $t^{th}$  iteration and to calculate this we need to add  $h_t$  to our previous prediction. So now we will apply this to our objective function

$$\begin{aligned} \text{obj}^{(t)} &= \sum_{i=1}^n L(y_i, F_t(x_i)) + \sum_{t=1}^T \Omega(h_t) \\ &= \sum_{i=1}^n L(y_i, F_{t-1}(x_i) + h_t(x_i)) + \sum_{t=1}^T \Omega(h_t) \end{aligned}$$

Here we greedily add the  $h_t$  that improves our model the most by minimizing our objective function. It acts as a **small update** to our final model.

In Gradient boosting algorithm we obtained  $F_t(x_i)$  at each iteration by **fitting a base learner to the negative gradient of the loss function with respect to previous iteration's value**.

In XGBoost, we explore several base learners/models and pick a model that minimizes the loss.

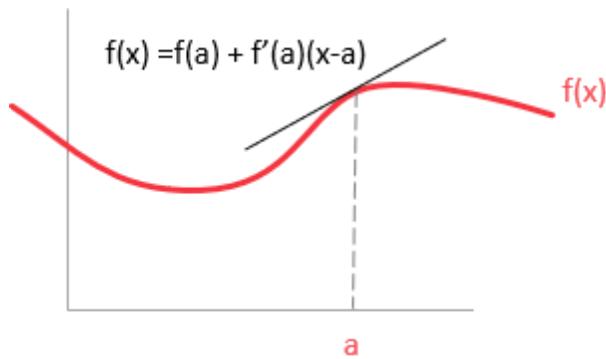
Our model  $h_t$  in XGBoost contains the structure of the tree and leaf scores, thus which seems a fairly complex optimization problem to be dealt with “Gradient descent” technique. This is due to the fact that an ensemble model includes “functions” as

value of the loss function for a base learner

## Taylor series approximation of the loss

The above described objective function can be approximated using Taylor series expansion and hence can be solved.

To have a better understanding, let's take a foot back and recall Taylor series from our calculus class.



Taylor approximation of a function around point  $a$ .

A Taylor series is a series expansion of a function about a point, Suppose that the function  $f(x)$  is infinitely differentiable(smooth) at  $x = a$ .

For  $f(x)$ ,  $\Delta x$  is the new learner we added in step  $t$  and  $a$  is the prediction at step ( $t-1$ )  $\Delta x = (x-a)$  is the new learner that we need to add in step ( $t$ ) in order to greedily minimize the objective.

By Taylor's expansion, any continuous function can be approximated by the linear combination of its first-order gradient and the quadratic function of the second-order



which can also be rephrased as:

$$f(x+h) = f(x) + \frac{f'(x)}{1!}(h) + \frac{f''(x)}{2!}(h)^2 + \frac{f'''(x)}{3!}(h)^3 + \dots,$$

by replacing  $a$  with  $x$  and  $x - a$  with  $h$ , where the function is continuous and n times differentiable in an interval  $[x, x + h]$

< >
Question 1/2
Mandatory

## Taylor Series

The Taylor series for the functions  $x^4 + x - 2$  which is differentiable at  $a = 1$  about the specified  $a$  is:

$5(x+1) + 6(x-1)^2 + 4(x+1)^3 + (x-1)^4$

$5(x-1) + 6(x-1)^2 + 4(x-1)^3 + (x-1)^4$

✓ Correct

Feedback:

$$f(x) = x^4 + x - 2.$$

$$f'(x) = 4x^3 + 1$$

$$f''(x) = 12x^2$$

$$f'''(x) = 24x$$



which is  $5(x - 1) + 6(x - 1)^2 + 4(x - 1)^3 + (x - 1)^4$

$(x - 1) + (x - 1)^2 + (x - 1)^3 + (x - 1)^4$

None of these



Your answer is Correct.

Attempt 1 of 2

Continue

So, in this case, we take Taylor expansion of the loss function up to the second order only and approximating the later differentiation terms to be  $\sim 0$ .

This will result in the objective function

$$\text{obj}^{(t)} = \sum_{i=1}^n L(y_i, F_{t-1}(x_i) + h_t(x_i)) + \sum_{t=1}^T \Omega(h_t)$$

as:

$$\text{obj}^{(t)} = \sum_{i=1}^n [L(y_i, F_{t-1}(x_i)) + p_i h_t(x_i) + \frac{1}{2} q_i h_t^2(x_i)] + \Omega(h_t)$$

where the  $p_i$  and  $q_i$  are defined as

$$p_i = \partial_{F_{t-1}(x_i)} L(y_i, F_{t-1}(x_i))$$

$$q_i = \partial_{F_{t-1}(x_i)}^2 L(y_i, F_{t-1}(x_i))$$



Hence, this becomes our optimization goal for the new tree. The advantage of this definition is that it only depends on  $p_i$  and  $q_i$  which also lets XGBoost support custom loss functions including logistic regression, weighted logistic regression etc.

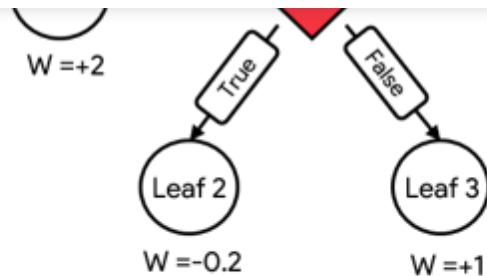
## XGBoost Regularisation

We have introduced the training step here, now what remained is defining the regularization term. Let's define the complexity of the tree  $\Omega(h_t)$ . In order to do so, let us first go through the definition of the tree  $h_t(x)$

$$h_t(x) = w_{m(x)}, w \in R^T, m : R^d \rightarrow \{1, 2, \dots, J_T\}$$

Here  $w$  is the vector of scores on leaves,  $m$  is a function (structure) assigning each data point to the corresponding leaf, and  $J_T$  is the number of leaves. Now the regularization function becomes:

$$\Omega(h_t) = \gamma * T + \frac{1}{2} * \lambda \sum_{j=1}^T w_j^2$$



$$\Omega(h_t) = \gamma * 3 + \frac{1}{2} \lambda (4 + 0.04 + 1)$$

An example of the complexity function for a tree carrying 3 leaves

## Further diving deep into XGBoost

Upon defining,  $I_j = \{i | m(x_i) = j\}$  as the instance set of leaf  $j$  and imputing the training and regularization part in the objective function, we can write it with the t-th tree as:

$$\begin{aligned}
 \text{obj}^{(t)} &\approx \sum_{i=1}^n [p_i w_{m(x_i)} + \frac{1}{2} q_i w_{m(x_i)}^2] + \gamma T + \frac{1}{2} \tau \sum_{j=1}^T w_j^2 \\
 &= \sum_{j=1}^T [(\sum_{i \in I_j} p_i) w_j + \frac{1}{2} (\sum_{i \in I_j} q_i + \tau) w_j^2] + \gamma T
 \end{aligned}$$

*Note: In the second line, the index of the summation has been changed because all the data points on the same leaf get the same score.*



$\sum_{j=1}^T \sum_{i=1}^{N_j} \sum_{k=1}^{n_j} \sum_{l=1}^{m_{jk}} \sum_{m=1}^{M_{ijk}}$

As  $w_j$ s are independent with respect to each other and  $P_j w_j + \frac{1}{2}(Q_j + \tau)w_j^2$  is a quadratic function hence for a fixed structure  $m(x)$ , we can compute the optimal weight  $w_j^*$  of leaf  $j$  as:

$$w_j^* = -\frac{P_j}{Q_j + \tau}$$

by differentiating the function  $P_j w_j + \frac{1}{2}(Q_j + \tau)w_j^2$  with respect to  $w_j$ .

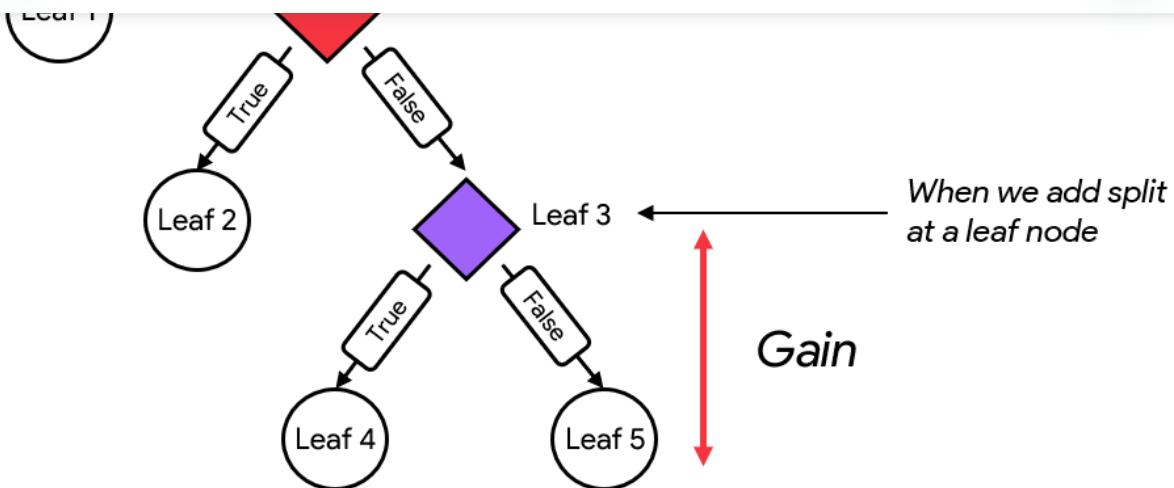
And, calculate the corresponding optimal value of the objective function by substituting the above-found  $w_j^*$  as

$$obj^* = -\frac{1}{2} \sum_{j=1}^T \frac{P_j^2}{Q_j + \tau} + \gamma T$$

*Note: The scoring function can be used as a measure of how good a tree structure  $m(x)$  is.*

It may sound a bit complicated but basically, for a given tree structure, we push the statistics

$p_i$  and  $q_i$  to the leaves they belong to and use the formula to calculate how good the tree is.



$$\text{obj} = -\frac{1}{2} \left[ \frac{P_1^2}{(Q_1 + \lambda)} + \frac{P_2^2}{(Q_2 + \lambda)} + \frac{P_3^2}{(Q_3 + \lambda)} \right] + \gamma * 3$$

$$\text{obj} = -\frac{1}{2} \left[ \frac{P_1^2}{(Q_1 + \lambda)} + \frac{P_2^2}{(Q_2 + \lambda)} + \frac{P_4^2}{(Q_4 + \lambda)} + \frac{P_5^2}{(Q_5 + \lambda)} \right] + \gamma * 4$$

$$\text{Gain} = \frac{1}{2} \left[ \frac{P_4^2}{(Q_4 + \lambda)} + \frac{P_5^2}{(Q_5 + \lambda)} - \frac{P_3^2}{(Q_3 + \lambda)} \right] - \gamma$$

$$\text{Gain} = \frac{1}{2} \left[ \frac{P_L^2}{(Q_L + \lambda)} + \frac{P_R^2}{(Q_R + \lambda)} - \frac{P_L^2 + P_R^2}{(Q_L + Q_R + \lambda)} \right] - \gamma$$

Based on some split criteria, the node is divided into left and right branches. Some instances fall in the left node and other instances fall in the right leaf node.

XGBoost greedily builds a tree. The split that results in maximum loss reduction or gain is chosen.

$$\text{Gain} = \text{Loss}(\text{parent}) - [\text{Loss}_L(\text{left branch}) + \text{Loss}_R(\text{right branch})]$$



reading material below.

### Additional References:

- Tianqi Chen explaining the XGBoost
- [XGBoost: A Scalable Tree Boosting System](#)
- [Finding the weights of a decision tree](#)
- [Complete Guide to Parameter Tuning in XGBoost](#)
- You can go through [this paper](#) for learning more about the Parallel Tree Learning Algorithm used for finding best split authored by the founder Tianqi Chen
- To have a better understanding of the objective function in the XGBoost scheme of things you can read from pg. 31 in the [following pdf](#)
- To read more about CatBoost, go through the [following paper](#) and the [following site](#)
- To read more about LightGBM which uses GOSS, refer the [following paper](#) and original documentation



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FINISH SESSION  
Mathematics behind  
XGBoost





which can also be rephrased as:

$$f(x + h) = f(x) + \frac{f'(x)}{1!}(h) + \frac{f''(x)}{2!}(h)^2 + \frac{f'''(x)}{3!}(h)^3 + \dots,$$

by replacing  $a$  with  $x$  and  $x - a$  with  $h$ , where the function is continuous and n times differentiable in an interval  $[x, x + h]$

<>Question 2/2Mandatory

✓

### Taylor Series

Given  $f(3) = 6$ ,  $f'(3) = 8$ ,  $f''(3) = 11$ , and all other higher order derivatives of  $f(x)$  are zero at  $x = 3$ , and assuming the function and all its derivatives exist and are continuous between  $x = 3$  and  $x = 7$ , the value of  $f(7)$  is

42

87.5

126

✓ Correct

! Feedback:  
The Taylor series is given by,



Upon substituting the respective values we'll get 126

231.5

✗ Incorrect



Feedback:

The Taylor series is given by,

$$f(x+h) = f(x) + \frac{f'(x)}{1!}(h) + \frac{f''(x)}{2!}(h)^2 + \frac{f'''(x)}{3!}(h)^3 + \dots,$$

$$x = 3, h = 7 - 3 = 4$$

$$f(7) = f(3) + f'(3).4 + \frac{f''(3)}{2}.4^2 + \frac{f'''(3)}{4}.4^3$$

Upon substituting the respective values what we'll get?

Your answer is Wrong.

Attempt 2 of 2

Continue

So, in this case, we take Taylor expansion of the loss function up to the second order only and approximating the later differentiation terms to be  $\sim 0$ .

This will result in the objective function

$$\text{obj}^{(t)} = \sum_{i=1}^n L(y_i, F_{t-1}(x_i) + h_t(x_i)) + \sum_{t=1}^T \Omega(h_t)$$

as:

$$\text{obj}^{(t)} = \sum_{i=1}^n [L(y_i, F_{t-1}(x_i)) + p_i h_t(x_i) + \frac{1}{2} q_i h_t^2(x_i)] + \Omega(h_t)$$