Gradient Boosting Machines (GBMs) with XGBoost

This tutorial is a part of Machine Learning with Python: Zero to GBMs and Zero to Data Science Bootcamp by Jovian

The following topics are covered in this tutorial:

- Downloading a real-world dataset from a Kaggle competition
- Performing feature engineering and prepare the dataset for training
- Training and interpreting a gradient boosting model using XGBoost
- Training with KFold cross validation and ensembling results
- Configuring the gradient boosting model and tuning hyperparamters

Let's begin by installing the required libraries.

```
#restart the kernel after installation
!pip install numpy pandas-profiling matplotlib seaborn --quiet
```

```
!pip install jovian opendatasets xgboost graphviz lightgbm scikit-learn xgboost lightgb
```

Problem Statement

This tutorial takes a practical and coding-focused approach. We'll learn gradient boosting by applying it to a real-world dataset from the Rossmann Store Sales competition on Kaggle:

> Rossmann operates over 3,000 drug stores in 7 European countries. Currently, Rossmann store managers are tasked with predicting their daily sales for up to six weeks in advance. Store sales are influenced by many factors, including promotions, competition, school and state holidays, seasonality, and locality.
>
> With thousands of individual managers predicting sales based on their unique circumstances, the accuracy of results can be quite varied. You are provided with historical sales data for 1,115 Rossmann stores. The task is to forecast the "Sales" column for the test set. Note that some stores in the dataset were temporarily closed for refurbishment.
>
> View and download the data here: https://www.kaggle.com/c/rossmann-store-sales/data

Downloading the Data

We can download the dataset from Kaggle directly within the Jupyter notebook using the `opendatasets` library. Make sure to accept the competition rules before executing the following cell.

```
import os
import opendatasets as od
import pandas as pd
pd.set_option("display.max_columns", 120)
pd.set_option("display.max_rows", 120)
```

```
od.download('https://www.kaggle.com/c/rossmann-store-sales')
```

```
Skipping, found downloaded files in "./rossmann-store-sales" (use force=True to force download)
```

You'll be asked to provide your Kaggle credentials to download the data. Follow these instructions: http://bit.ly/kaggle-creds

```
os.listdir('rossmann-store-sales')
```

```
['test.csv', 'train.csv', 'store.csv', 'sample_submission.csv']
```

Let's load the data into Pandas dataframes.

```
ross_df = pd.read_csv('./rossmann-store-sales/train.csv', low_memory=False)
store_df = pd.read_csv('./rossmann-store-sales/store.csv')
test_df = pd.read_csv('./rossmann-store-sales/test.csv')
submission_df = pd.read_csv('./rossmann-store-sales/sample_submission.csv')
```

```
ross_df
```

	Store	DayOfWeek	Date	Sales	Customers	Open	Promo	StateHoliday	SchoolHoliday
0	1	5	2015-07-31	5263	555	1	1	0	1
1	2	5	2015-07-31	6064	625	1	1	0	1
2	3	5	2015-07-31	8314	821	1	1	0	1
3	4	5	2015-07-31	13995	1498	1	1	0	1
4	5	5	2015-07-31	4822	559	1	1	0	1
...	...	...	...	...	...	...	...	...	...
1017204	1111	2	2013-01-01	0	0	0	0	a	1
1017205	1112	2	2013-01-01	0	0	0	0	a	1
1017206	1113	2	2013-01-01	0	0	0	0	a	1
1017207	1114	2	2013-01-01	0	0	0	0	a	1
1017208	1115	2	2013-01-01	0	0	0	0	a	1

1017209 rows × 9 columns

```
test_df
```

	Id	Store	DayOfWeek	Date	Open	Promo	StateHoliday	SchoolHoliday
0	1	1	4	2015-09-17	1.0	1	0	0
1	2	3	4	2015-09-17	1.0	1	0	0
2	3	7	4	2015-09-17	1.0	1	0	0
3	4	8	4	2015-09-17	1.0	1	0	0
4	5	9	4	2015-09-17	1.0	1	0	0
...	...	...	...	...	...	...	...	...
41083	41084	1111	6	2015-08-01	1.0	0	0	0
41084	41085	1112	6	2015-08-01	1.0	0	0	0
41085	41086	1113	6	2015-08-01	1.0	0	0	0
41086	41087	1114	6	2015-08-01	1.0	0	0	0
41087	41088	1115	6	2015-08-01	1.0	0	0	1

41088 rows × 8 columns

```
submission_df
```

	Id	Sales
0	1	0
1	2	0
2	3	0
3	4	0
4	5	0
...	...	...
41083	41084	0
41084	41085	0
41085	41086	0
41086	41087	0
41087	41088	0

41088 rows × 2 columns

```
store_df
```

	Store	StoreType	Assortment	CompetitionDistance	CompetitionOpenSinceMonth	CompetitionOpenSinceYear	Pro
0	1	c	a	1270.0	9.0	2008.0	
1	2	a	a	570.0	11.0	2007.0	
2	3	a	a	14130.0	12.0	2006.0	
3	4	c	c	620.0	9.0	2009.0	

	Store	StoreType	Assortment	CompetitionDistance	CompetitionOpenSinceMonth	CompetitionOpenSinceYear	Pro
4	5	a	a	29910.0	4.0	2015.0	
...	...	...	...	...	...	...	
1110	1111	a	a	1900.0	6.0	2014.0	
1111	1112	c	c	1880.0	4.0	2006.0	
1112	1113	a	c	9260.0	NaN	NaN	
1113	1114	a	c	870.0	NaN	NaN	
1114	1115	d	c	5350.0	NaN	NaN	

1115 rows × 10 columns

> **EXERCISE**: Read the data description provided on the competition page to understand what the values in each column of `store_df` represent.

Let's merge the information from `store_df` into `train_df` and `test_df`.

```
merged_df = ross_df.merge(store_df, how='left', on='Store')
merged_test_df = test_df.merge(store_df, how='left', on='Store')
```

```
merged_df
```

	Store	DayOfWeek	Date	Sales	Customers	Open	Promo	StateHoliday	SchoolHoliday	StoreType	Assor
0	1	5	2015-07-31	5263	555	1	1	0	1	c	
1	2	5	2015-07-31	6064	625	1	1	0	1	a	
2	3	5	2015-07-31	8314	821	1	1	0	1	a	
3	4	5	2015-07-31	13995	1498	1	1	0	1	c	
4	5	5	2015-07-31	4822	559	1	1	0	1	a	
...	...	...	...	...	...	...	...	...	...	...	
1017204	1111	2	2013-01-01	0	0	0	0	a	1	a	
1017205	1112	2	2013-01-01	0	0	0	0	a	1	c	
1017206	1113	2	2013-01-01	0	0	0	0	a	1	a	
1017207	1114	2	2013-01-01	0	0	0	0	a	1	a	
1017208	1115	2	2013-01-01	0	0	0	0	a	1	d	

1017209 rows × 18 columns

> **EXERCISE**: Perform exploratory data analysis and visualization on the dataset. Study the distribution of values in each column, and their relationship with the target column `Sales`.

```
```

```
```

Let's save our work before continuing.

```
jovian.commit()
```

```
[jovian] Committed successfully! https://jovian.ai/aakashns/python-gradient-boosting-machines
```

```
'https://jovian.ai/aakashns/python-gradient-boosting-machines'
```

Preprocessing and Feature Engineering

Let's take a look at the available columns, and figure out if we can create new columns or apply any useful transformations.

```
merged_df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 1017209 entries, 0 to 1017208
Data columns (total 18 columns):
 #   Column                     Non-Null Count    Dtype  
---  ------                     --------------    -----  
 0   Store                      1017209 non-null  int64  
 1   DayOfWeek                  1017209 non-null  int64  
 2   Date                       1017209 non-null  object 
 3   Sales                      1017209 non-null  int64  
 4   Customers                  1017209 non-null  int64  
 5   Open                       1017209 non-null  int64  
 6   Promo                      1017209 non-null  int64  
 7   StateHoliday               1017209 non-null  object 
 8   SchoolHoliday              1017209 non-null  int64  
 9   StoreType                  1017209 non-null  object 
 10  Assortment                 1017209 non-null  object 
 11  CompetitionDistance        1014567 non-null  float64
 12  CompetitionOpenSinceMonth  693861 non-null   float64
 13  CompetitionOpenSinceYear   693861 non-null   float64
```

```
 14  Promo2                     1017209 non-null  int64
 15  Promo2SinceWeek            509178 non-null   float64
 16  Promo2SinceYear            509178 non-null   float64
 17  PromoInterval              509178 non-null   object
dtypes: float64(5), int64(8), object(5)
memory usage: 147.5+ MB
```

Date

First, let's convert `Date` to a `date`column and extract different parts of the date.

```
def split_date(df):
    df['Date'] = pd.to_datetime(df['Date'])
    df['Year'] = df.Date.dt.year
    df['Month'] = df.Date.dt.month
    df['Day'] = df.Date.dt.day
    df['WeekOfYear'] = df.Date.dt.isocalendar().week
```

```
split_date(merged_df)
split_date(merged_test_df)
```

```
merged_df
```

	Store	DayOfWeek	Date	Sales	Customers	Open	Promo	StateHoliday	SchoolHoliday	StoreType	Asso
0	1	5	2015-07-31	5263	555	1	1	0	1	c	
1	2	5	2015-07-31	6064	625	1	1	0	1	a	
2	3	5	2015-07-31	8314	821	1	1	0	1	a	
3	4	5	2015-07-31	13995	1498	1	1	0	1	c	
4	5	5	2015-07-31	4822	559	1	1	0	1	a	
...	...	...	...	...	...	...	...	...	...	...	
1017204	1111	2	2013-01-01	0	0	0	0	a	1	a	
1017205	1112	2	2013-01-01	0	0	0	0	a	1	c	
1017206	1113	2	2013-01-01	0	0	0	0	a	1	a	
1017207	1114	2	2013-01-01	0	0	0	0	a	1	a	
1017208	1115	2	2013-01-01	0	0	0	0	a	1	d	

1017209 rows × 22 columns

Store Open/Closed

Next, notice that the sales are zero whenever the store is closed.

```
merged_df[merged_df.Open == 0].Sales.value_counts()
```

```
0    172817
Name: Sales, dtype: int64
```

Instead of trying to model this relationship, it would be better to hard-code it in our predictions, and remove the rows where the store is closed. We won't remove any rows from the test set, since we need to make predictions for every row.

```
merged_df = merged_df[merged_df.Open == 1].copy()
```

Competition

Next, we can use the columns `CompetitionOpenSince[Month/Year]` columns from `store_df` to compute the number of months for which a competitor has been open near the store.

```
def comp_months(df):
    df['CompetitionOpen'] = 12 * (df.Year - df.CompetitionOpenSinceYear) + (df.Month -
    df['CompetitionOpen'] = df['CompetitionOpen'].map(lambda x: 0 if x < 0 else x).fill
```

```
comp_months(merged_df)
comp_months(merged_test_df)
```

```
merged_df
```

	Store	DayOfWeek	Date	Sales	Customers	Open	Promo	StateHoliday	SchoolHoliday	StoreType	Asso
0	1	5	2015-07-31	5263	555	1	1	0	1	c	
1	2	5	2015-07-31	6064	625	1	1	0	1	a	
2	3	5	2015-07-31	8314	821	1	1	0	1	a	
3	4	5	2015-07-31	13995	1498	1	1	0	1	c	
4	5	5	2015-07-31	4822	559	1	1	0	1	a	
...	...	...	...	...	...	...	...	...	...	...	
1016776	682	2	2013-01-01	3375	566	1	0	a	1	b	
1016827	733	2	2013-01-01	10765	2377	1	0	a	1	b	
1016863	769	2	2013-01-01	5035	1248	1	0	a	1	b	
1017042	948	2	2013-01-01	4491	1039	1	0	a	1	b	
1017190	1097	2	2013-01-01	5961	1405	1	0	a	1	b	

844392 rows × 23 columns

Let's view the results of the new columns we've created.

```
merged_df[['Date', 'CompetitionDistance', 'CompetitionOpenSinceYear', 'CompetitionOpenS
```

	Date	CompetitionDistance	CompetitionOpenSinceYear	CompetitionOpenSinceMonth	CompetitionOpen
21092	2015-07-13	3740.0	2002.0	2.0	161.0
521375	2014-03-21	190.0	2011.0	9.0	30.0
962441	2013-02-19	21930.0	NaN	NaN	0.0
572789	2014-02-03	10890.0	2005.0	4.0	106.0
744556	2013-09-02	7160.0	2012.0	11.0	10.0
375144	2014-08-05	3390.0	NaN	NaN	0.0
339654	2014-09-12	1850.0	2014.0	12.0	0.0
79686	2015-05-21	7160.0	2012.0	11.0	30.0
853087	2013-05-28	18540.0	NaN	NaN	0.0
91114	2015-05-11	2020.0	2014.0	7.0	10.0
798663	2013-07-16	3490.0	2011.0	4.0	27.0
651052	2013-11-25	3250.0	NaN	NaN	0.0
222496	2015-01-13	2490.0	2012.0	11.0	26.0
76973	2015-05-23	260.0	2006.0	10.0	103.0
934911	2013-03-15	15050.0	2008.0	9.0	54.0
846182	2013-06-03	2850.0	2014.0	7.0	0.0
361565	2014-08-20	2480.0	1990.0	7.0	289.0
774624	2013-08-06	3270.0	NaN	NaN	0.0
708076	2013-10-05	14600.0	2015.0	4.0	0.0
376588	2014-08-04	3350.0	NaN	NaN	0.0

Additional Promotion

We can also add some additional columns to indicate how long a store has been running `Promo2` and whether a new round of `Promo2` starts in the current month.

```
def check_promo_month(row):
    month2str = {1:'Jan', 2:'Feb', 3:'Mar', 4:'Apr', 5:'May', 6:'Jun',
                 7:'Jul', 8:'Aug', 9:'Sept', 10:'Oct', 11:'Nov', 12:'Dec'}
    try:
        months = (row['PromoInterval'] or '').split(',')
        if row['Promo2Open'] and month2str[row['Month']] in months:
            return 1
        else:
            return 0
    except Exception:
        return 0
```

```
def promo_cols(df):
    # Months since Promo2 was open
    df['Promo2Open'] = 12 * (df.Year - df.Promo2SinceYear) +  (df.WeekOfYear - df.Promo
    df['Promo2Open'] = df['Promo2Open'].map(lambda x: 0 if x < 0 else x).fillna(0) * df
    # Whether a new round of promotions was started in the current month
    df['IsPromo2Month'] = df.apply(check_promo_month, axis=1) * df['Promo2']
```

```
promo_cols(merged_df)
promo_cols(merged_test_df)
```

Let's view the results of the columns we've created.

```
merged_df[['Date', 'Promo2', 'Promo2SinceYear', 'Promo2SinceWeek', 'PromoInterval', 'Pr
```

	Date	Promo2	Promo2SinceYear	Promo2SinceWeek	PromoInterval	Promo2Open	IsPromo2Month
271634	2014-11-24	1	2011.0	18.0	Feb,May,Aug,Nov	42.885246	1
66318	2015-06-02	1	2009.0	45.0	Jan,Apr,Jul,Oct	66.950820	0
63049	2015-06-05	0	NaN	NaN	NaN	0.000000	0
588334	2014-01-20	1	2011.0	14.0	Jan,Apr,Jul,Oct	33.704918	1
500994	2014-04-08	1	2014.0	10.0	Mar,Jun,Sept,Dec	1.147541	0
79333	2015-05-21	1	2014.0	18.0	Feb,May,Aug,Nov	12.688525	1
396138	2014-07-14	1	2013.0	36.0	Jan,Apr,Jul,Oct	10.393443	1
540035	2014-03-04	1	2011.0	14.0	Jan,Apr,Jul,Oct	35.081967	0
723881	2013-09-21	1	2012.0	40.0	Jan,Apr,Jul,Oct	11.540984	0
435210	2014-06-06	0	NaN	NaN	NaN	0.000000	0
346549	2014-09-05	0	NaN	NaN	NaN	0.000000	0
150873	2015-03-18	0	NaN	NaN	NaN	0.000000	0
835446	2013-06-13	0	NaN	NaN	NaN	0.000000	0
656786	2013-11-20	0	NaN	NaN	NaN	0.000000	0
297087	2014-10-28	0	NaN	NaN	NaN	0.000000	0
654882	2013-11-21	0	NaN	NaN	NaN	0.000000	0
684054	2013-10-26	0	NaN	NaN	NaN	0.000000	0
111620	2015-04-22	1	2013.0	36.0	Mar,Jun,Sept,Dec	19.639344	0
767206	2013-08-13	1	2015.0	23.0	Mar,Jun,Sept,Dec	0.000000	0
613772	2013-12-28	0	NaN	NaN	NaN	0.000000	0

The features related to competition and promotion are now much more useful.

Input and Target Columns

Let's select the columns that we'll use for training.

```
merged_df.columns
```

```
Index(['Store', 'DayOfWeek', 'Date', 'Sales', 'Customers', 'Open', 'Promo',
```

```
       'StateHoliday', 'SchoolHoliday', 'StoreType', 'Assortment',
       'CompetitionDistance', 'CompetitionOpenSinceMonth',
       'CompetitionOpenSinceYear', 'Promo2', 'Promo2SinceWeek',
       'Promo2SinceYear', 'PromoInterval', 'Year', 'Month', 'Day',
       'WeekOfYear', 'CompetitionOpen', 'Promo2Open', 'IsPromo2Month'],
      dtype='object')
```

```
input_cols = ['Store', 'DayOfWeek', 'Promo', 'StateHoliday', 'SchoolHoliday',
              'StoreType', 'Assortment', 'CompetitionDistance', 'CompetitionOpen',
              'Day', 'Month', 'Year', 'WeekOfYear',  'Promo2',
              'Promo2Open', 'IsPromo2Month']
target_col = 'Sales'
```

```
inputs = merged_df[input_cols].copy()
targets = merged_df[target_col].copy()
```

```
test_inputs = merged_test_df[input_cols].copy()
```

Let's also identify numeric and categorical columns. Note that we can treat binary categorical columns (0/1) as numeric columns.

```
numeric_cols = ['Store', 'Promo', 'SchoolHoliday',
              'CompetitionDistance', 'CompetitionOpen', 'Promo2', 'Promo2Open', 'IsProm
              'Day', 'Month', 'Year', 'WeekOfYear',  ]
categorical_cols = ['DayOfWeek', 'StateHoliday', 'StoreType', 'Assortment']
```

Impute missing numerical data

```
inputs[numeric_cols].isna().sum()
```

```
Store                 0
Promo                 0
SchoolHoliday         0
CompetitionDistance    0
CompetitionOpen       0
Promo2                0
Promo2Open            0
IsPromo2Month         0
Day                   0
Month                 0
Year                  0
WeekOfYear            0
dtype: int64
```

```
test_inputs[numeric_cols].isna().sum()
```

```
Store                 0
Promo                 0
```

```
SchoolHoliday            0
CompetitionDistance      0
CompetitionOpen          0
Promo2                   0
Promo2Open               0
IsPromo2Month            0
Day                      0
Month                    0
Year                     0
WeekOfYear               0
dtype: int64
```

Seems like competition distance is the only missing value, and we can simply fill it with the highest value (to indicate that competition is very far away).

```
max_distance = inputs.CompetitionDistance.max()
```

```
inputs['CompetitionDistance'].fillna(max_distance, inplace=True)
test_inputs['CompetitionDistance'].fillna(max_distance, inplace=True)
```

Scale Numeric Values

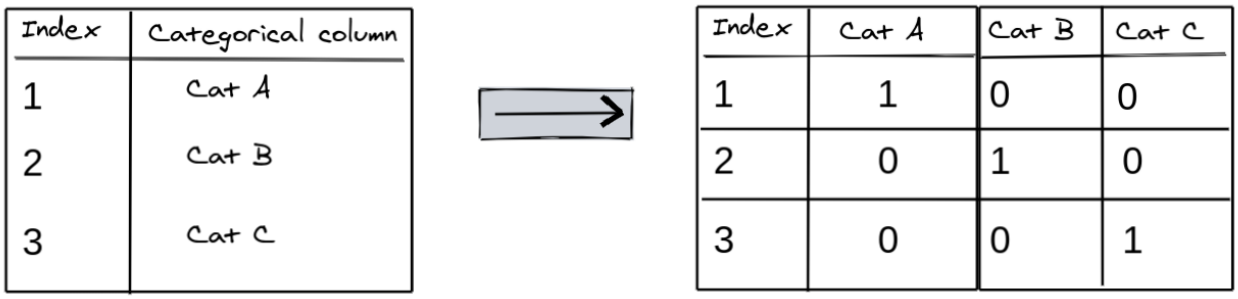
Let's scale numeric values to the 0 to 1 range.

```
from sklearn.preprocessing import MinMaxScaler
```

```
scaler = MinMaxScaler().fit(inputs[numeric_cols])
```

```
inputs[numeric_cols] = scaler.transform(inputs[numeric_cols])
test_inputs[numeric_cols] = scaler.transform(test_inputs[numeric_cols])
```

Encode Categorical Columns



Let's one-hot encode categorical columns.

```
from sklearn.preprocessing import OneHotEncoder
```

```
encoder = OneHotEncoder(sparse=False, handle_unknown='ignore').fit(inputs[categorical_c
encoded_cols = list(encoder.get_feature_names(categorical_cols))
```

```
inputs[encoded_cols] = encoder.transform(inputs[categorical_cols])
test_inputs[encoded_cols] = encoder.transform(test_inputs[categorical_cols])
```

Finally, let's extract out all the numeric data for training.

```
X = inputs[numeric_cols + encoded_cols]
X_test = test_inputs[numeric_cols + encoded_cols]
```

We haven't created a validation set yet, because we'll use K-fold cross validation.

> **EXERCISE**: Look through the notebooks created by participants in the Kaggle competition and apply some other ideas for feature engineering. https://www.kaggle.com/c/rossmann-store-sales/code?competitionId=4594&sortBy=voteCount

```

```

```

```

Let's save our work before continuing.

```
jovian.commit()
```

```
[jovian] Updating notebook "aakashns/python-gradient-boosting-machines" on https://jovian.ai/
[jovian] Committed successfully! https://jovian.ai/aakashns/python-gradient-boosting-machines
```

```
'https://jovian.ai/aakashns/python-gradient-boosting-machines'
```

Gradient Boosting

We're now ready to train our gradient boosting machine (GBM) model. Here's how a GBM model works:

1. The average value of the target column and uses as an initial prediction every input.
2. The residuals (difference) of the predictions with the targets are computed.
3. A decision tree of limited depth is trained to **predict just the residuals** for each input.
4. Predictions from the decision tree are scaled using a parameter called the learning rate (this prevents overfitting)
5. Scaled predictions fro the tree are added to the previous predictions to obtain the new and improved predictions.

6. Steps 2 to 5 are repeated to create new decision trees, each of which is trained to predict just the residuals from the previous prediction.

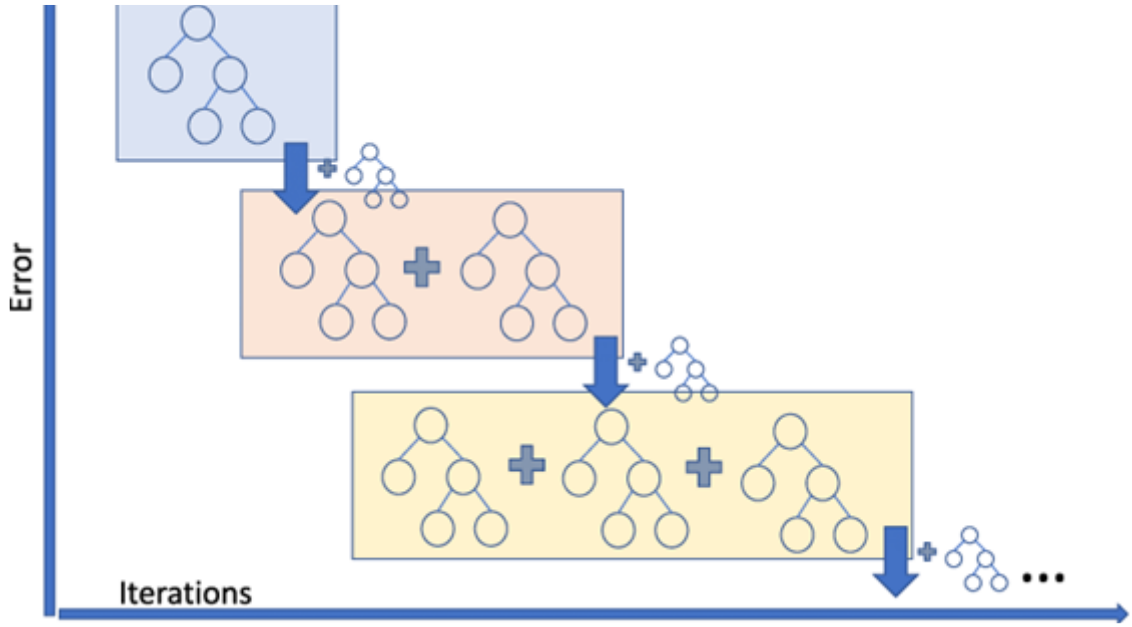
The term "gradient" refers to the fact that each decision tree is trained with the purpose of reducing the loss from the previous iteration (similar to gradient descent). The term "boosting" refers the general technique of training new models to improve the results of an existing model.

> **EXERCISE**: Can you describe in your own words how a gradient boosting machine is different from a random forest?

For a mathematical explanation of gradient boosting, check out the following resources:

- XGBoost Documentation
- Video Tutorials on StatQuest

Here's a visual representation of gradient boosting:



Training

To train a GBM, we can use the `XGBRegressor` class from the `XGBoost` library.

```
from xgboost import XGBRegressor
```

```
?XGBRegressor
```

```
model = XGBRegressor(random_state=42, n_jobs=-1, n_estimators=20, max_depth=4)
```

Let's train the model using `model.fit` .

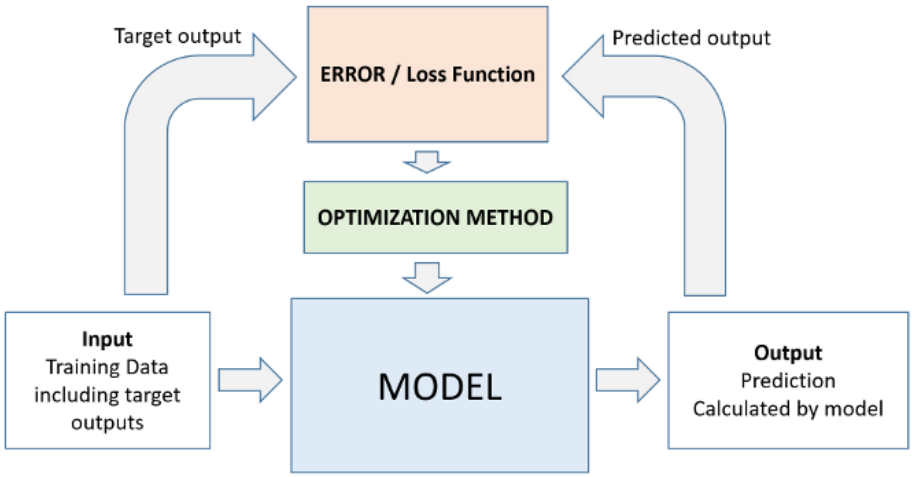
```
%%time
model.fit(X, targets)
```

```
CPU times: user 44.7 s, sys: 1.53 s, total: 46.2 s
```

```
Wall time: 3.23 s
```

```
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=4,
             min_child_weight=1, missing=nan, monotone_constraints='()',
             n_estimators=20, n_jobs=-1, num_parallel_tree=1, random_state=42,
             reg_alpha=0, reg_lambda=1, scale_pos_weight=1, subsample=1,
             tree_method='exact', validate_parameters=1, verbosity=None)
```

> **EXERCISE**: Explain how the `.fit` method of `XGBRegressor` applies the iterative machine learning workflow to train the model using the training data.



Prediction

We can now make predictions and evaluate the model using `model.predict`.

```
preds = model.predict(X)
```

```
preds
```

```
array([ 8127.9404,  7606.919 ,  8525.857 , ...,  6412.8247,  9460.068 ,
       10302.145 ], dtype=float32)
```

Evaluation

Let's evaluate the predictions using RMSE error.

```
from sklearn.metrics import mean_squared_error

def rmse(a, b):
    return mean_squared_error(a, b, squared=False)
```

```
rmse(preds, targets)
```

```
2377.752008804669
```

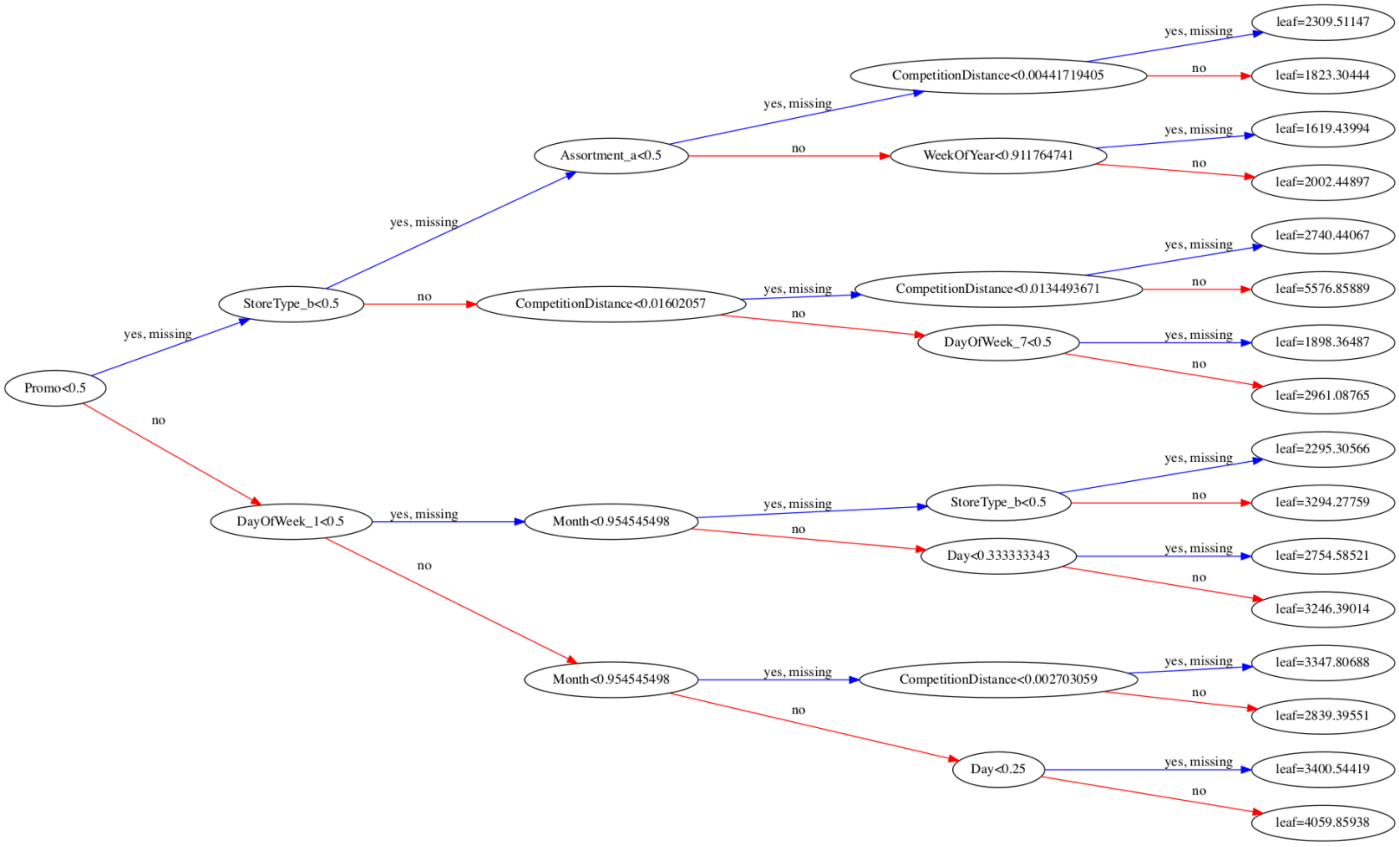
Visualization

We can visualize individual trees using `plot_tree` (note: this requires the `graphviz` library to be installed).

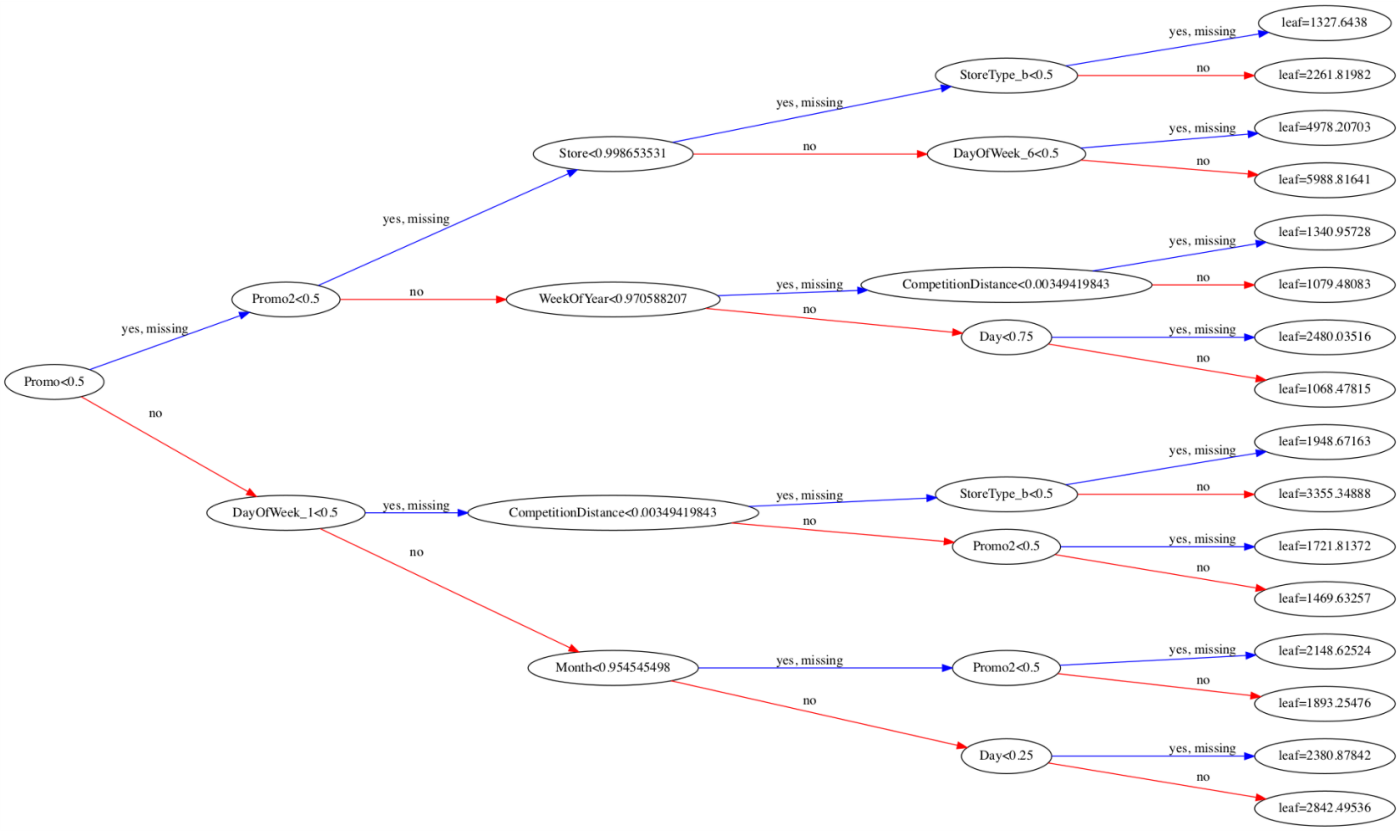
```
import matplotlib.pyplot as plt
from xgboost import plot_tree
from matplotlib.pylab import rcParams
%matplotlib inline

rcParams['figure.figsize'] = 30,30
```

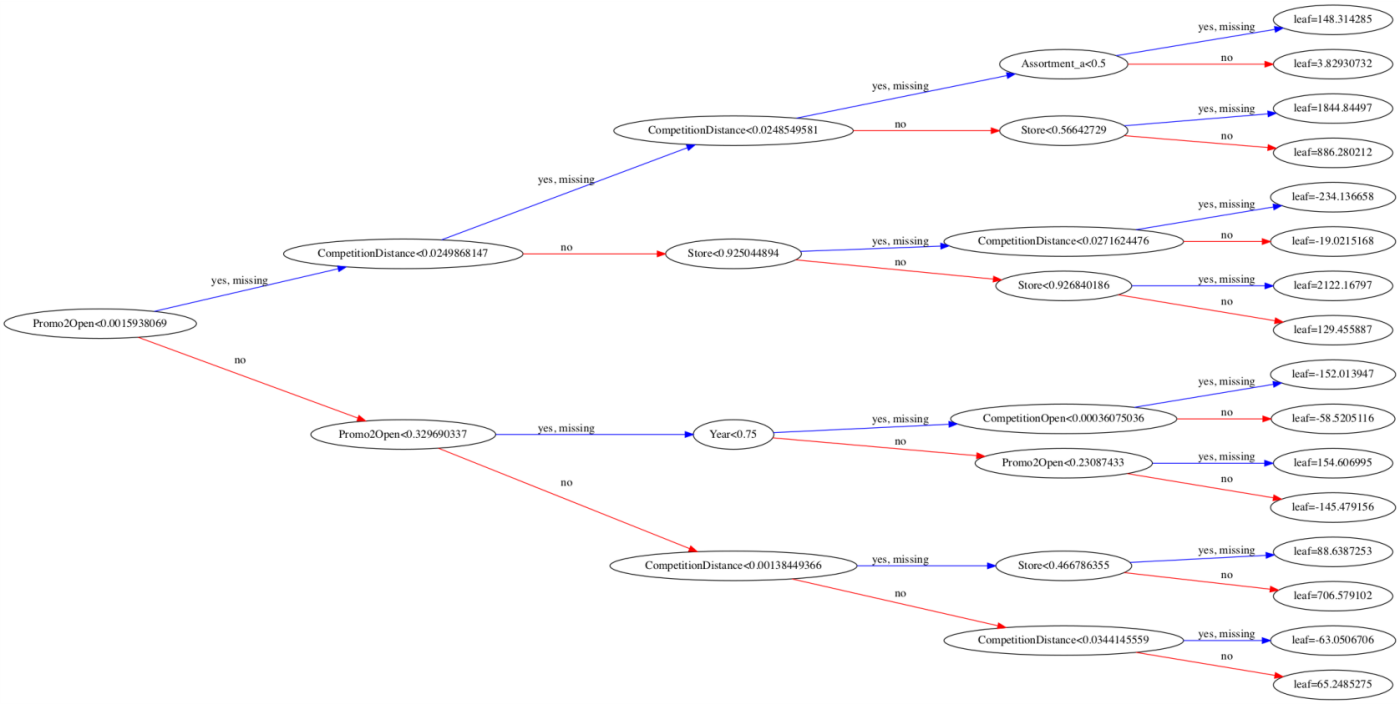
```
plot_tree(model, rankdir='LR');
```




```
plot_tree(model, rankdir='LR', num_trees=1);
```




```
plot_tree(model, rankdir='LR', num_trees=19);
```



Notice how the trees only compute residuals, and not the actual target value. We can also visualize the tree as text.

```
trees = model.get_booster().get_dump()
```

```
len(trees)
```

```
20
```

```
print(trees[0])
```

```
0:[Promo<0.5] yes=1,no=2,missing=1
    1:[StoreType_b<0.5] yes=3,no=4,missing=3
        3:[Assortment_a<0.5] yes=7,no=8,missing=7
            7:[CompetitionDistance<0.00441719405] yes=15,no=16,missing=15
                15:leaf=2309.51147
                16:leaf=1823.30444
            8:[WeekOfYear<0.911764741] yes=17,no=18,missing=17
                17:leaf=1619.43994
                18:leaf=2002.44897
        4:[CompetitionDistance<0.01602057] yes=9,no=10,missing=9
            9:[CompetitionDistance<0.0134493671] yes=19,no=20,missing=19
                19:leaf=2740.44067
                20:leaf=5576.85889
            10:[DayOfWeek_7<0.5] yes=21,no=22,missing=21
                21:leaf=1898.36487
                22:leaf=2961.08765
    2:[DayOfWeek_1<0.5] yes=5,no=6,missing=5
        5:[Month<0.954545498] yes=11,no=12,missing=11
            11:[StoreType_b<0.5] yes=23,no=24,missing=23
                23:leaf=2295.30566
                24:leaf=3294.27759
            12:[Day<0.333333343] yes=25,no=26,missing=25
                25:leaf=2754.58521
                26:leaf=3246.39014
        6:[Month<0.954545498] yes=13,no=14,missing=13
            13:[CompetitionDistance<0.002703059] yes=27,no=28,missing=27
                27:leaf=3347.80688
                28:leaf=2839.39551
            14:[Day<0.25] yes=29,no=30,missing=29
                29:leaf=3400.54419
                30:leaf=4059.85938
```

Feature importance

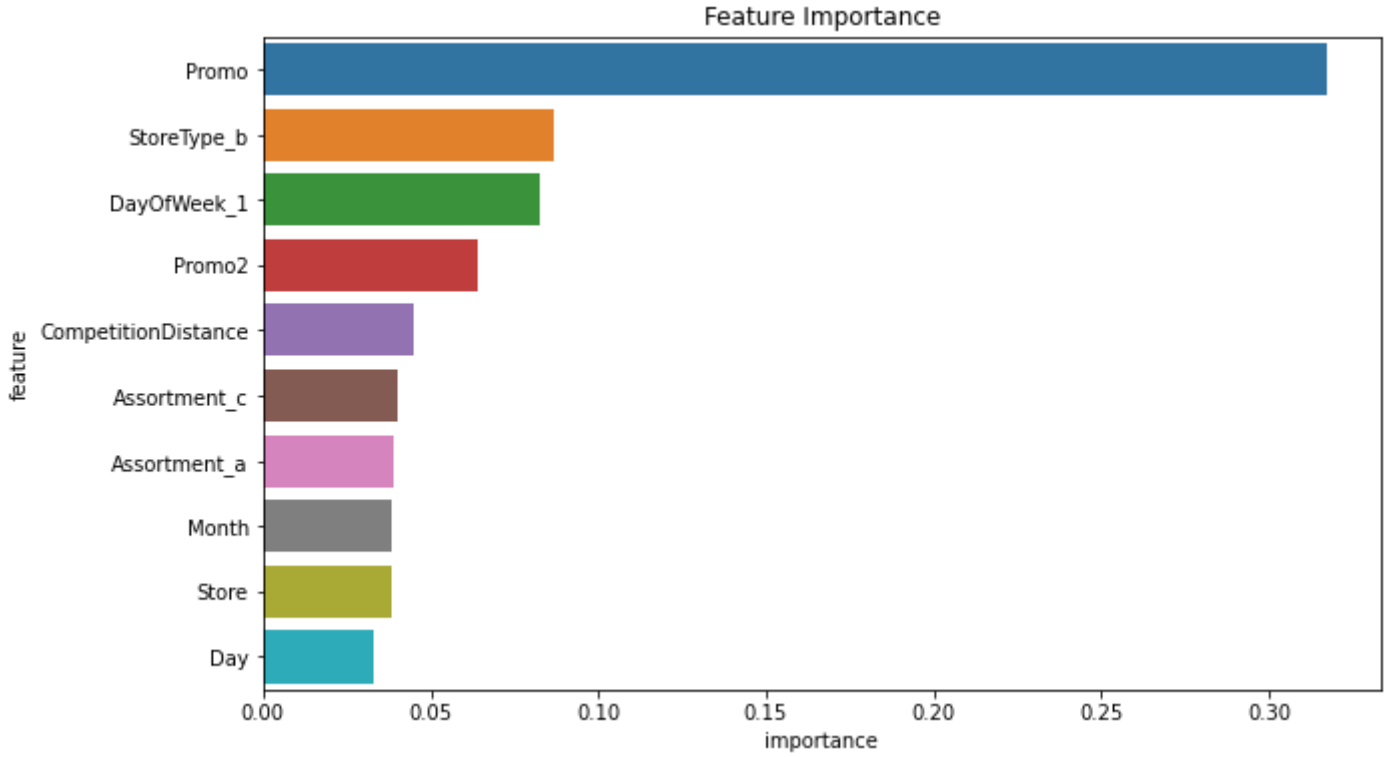
Just like decision trees and random forests, XGBoost also provides a feature importance score for each column in the input.

```
importance_df = pd.DataFrame({
    'feature': X.columns,
    'importance': model.feature_importances_
}).sort_values('importance', ascending=False)
```

```
importance_df.head(10)
```

	feature	importance
1	Promo	0.317473
24	StoreType_b	0.086472
12	DayOfWeek_1	0.082269
5	Promo2	0.063986
3	CompetitionDistance	0.045053
29	Assortment_c	0.040226
27	Assortment_a	0.038759
9	Month	0.038493
0	Store	0.038119
8	Day	0.033209

```
import seaborn as sns
plt.figure(figsize=(10,6))
plt.title('Feature Importance')
sns.barplot(data=importance_df.head(10), x='importance', y='feature');
```



Let's save our work before continuing.

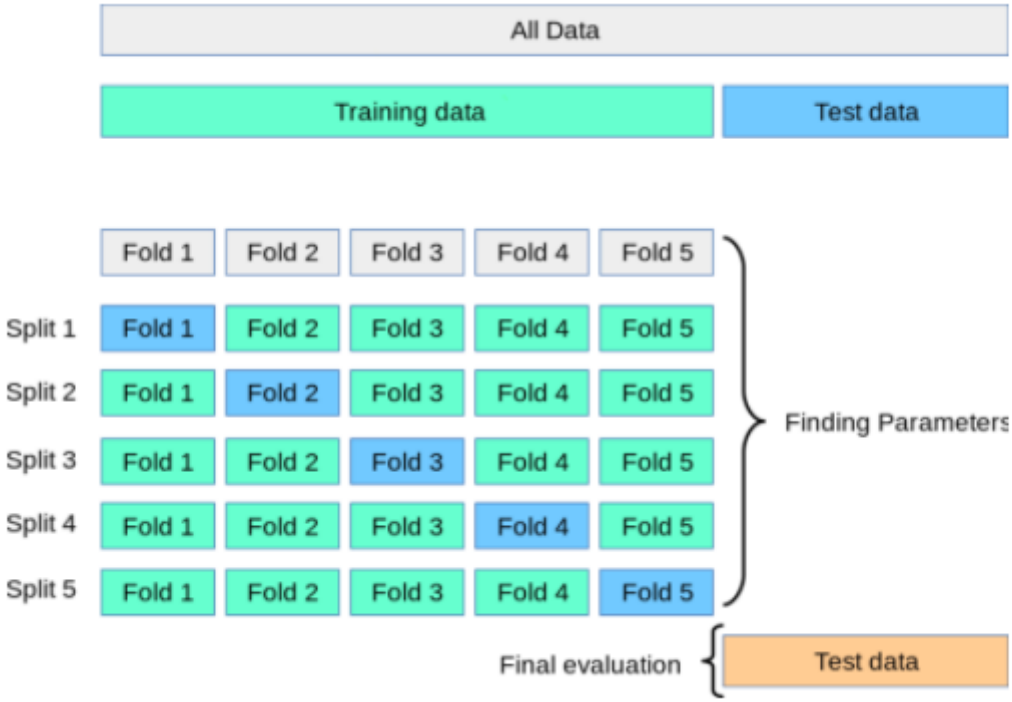
```
jovian.commit()
```

```
[jovian] Updating notebook "aakashns/python-gradient-boosting-machines" on https://jovian.ai/
[jovian] Committed successfully! https://jovian.ai/aakashns/python-gradient-boosting-machines
```

```
'https://jovian.ai/aakashns/python-gradient-boosting-machines'
```

K Fold Cross Validation

Notice that we didn't create a validation set before training our XGBoost model. We'll use a different validation strategy this time, called K-fold cross validation (source):



Scikit-learn provides utilities for performing K fold cross validation.

```
from sklearn.model_selection import KFold
```

Let's define a helper function `train_and_evaluate` which trains a model the given parameters and returns the trained model, training error and validation error.

```
def train_and_evaluate(X_train, train_targets, X_val, val_targets, **params):
    model = XGBRegressor(random_state=42, n_jobs=-1, **params)
    model.fit(X_train, train_targets)
    train_rmse = rmse(model.predict(X_train), train_targets)
    val_rmse = rmse(model.predict(X_val), val_targets)
    return model, train_rmse, val_rmse
```

Now, we can use the `KFold` utility to create the different training/validations splits and train a separate model for each fold.

```
kfold = KFold(n_splits=5)
```

```
models = []

for train_idxs, val_idxs in kfold.split(X):
    X_train, train_targets = X.iloc[train_idxs], targets.iloc[train_idxs]
```

```
    X_val, val_targets = X.iloc[val_idxs], targets.iloc[val_idxs]
    model, train_rmse, val_rmse = train_and_evaluate(X_train,
                                                     train_targets,
                                                     X_val,
                                                     val_targets,
                                                     max_depth=4,
                                                     n_estimators=20)
    models.append(model)
    print('Train RMSE: {}, Validation RMSE: {}'.format(train_rmse, val_rmse))
```

```
Train RMSE: 2352.216448531526, Validation RMSE: 2424.6228916973314
Train RMSE: 2406.709513789309, Validation RMSE: 2451.9646038059277
Train RMSE: 2365.7354745443067, Validation RMSE: 2336.984157073758
Train RMSE: 2366.4732092777763, Validation RMSE: 2460.8995475901697
Train RMSE: 2379.3752997474626, Validation RMSE: 2440.665320626728
```

Let's also define a function to average predictions from the 5 different models.

```
import numpy as np

def predict_avg(models, inputs):
    return np.mean([model.predict(inputs) for model in models], axis=0)
```

```
preds = predict_avg(models, X)
```

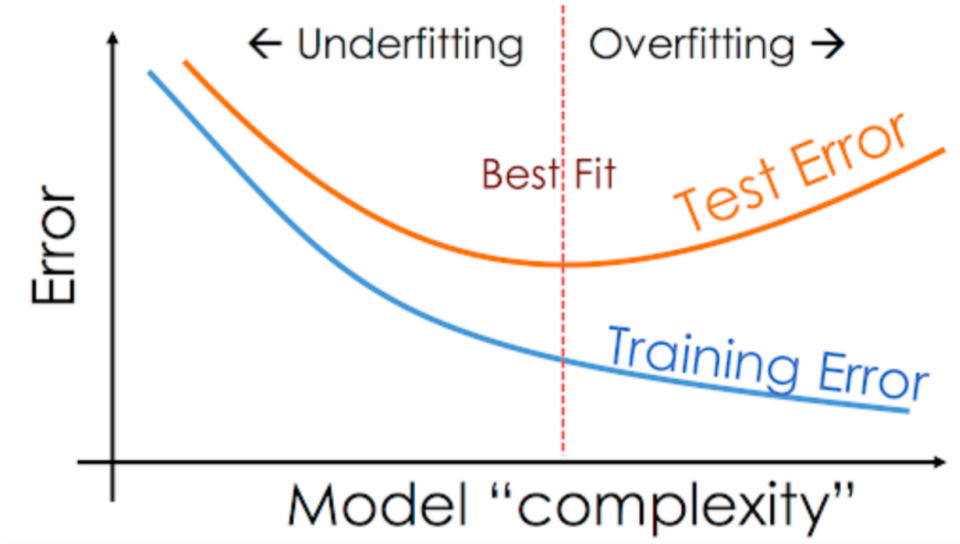
```
preds
```

```
array([8021.374 , 7577.715 , 8747.863 , ..., 7615.0303, 7924.784 ,
       9600.297 ], dtype=float32)
```

We can now use `predict_avg` to make predictions for the test set.

Hyperparameter Tuning and Regularization

Just like other machine learning models, there are several hyperparameters we can to adjust the capacity of model and reduce overfitting.



Check out the following resources to learn more about hyperparameter supported by XGBoost:

- https://xgboost.readthedocs.io/en/latest/python/python_api.html#xgboost.XGBRegressor
- https://xgboost.readthedocs.io/en/latest/parameter.html

```
model
```

```
?XGBRegressor
```

Here's a helper function to test hyperparameters with K-fold cross validation.

```
def test_params_kfold(n_splits, **params):
    train_rmses, val_rmses, models = [], [], []
    kfold = KFold(n_splits)
    for train_idxs, val_idxs in kfold.split(X):
        X_train, train_targets = X.iloc[train_idxs], targets.iloc[train_idxs]
        X_val, val_targets = X.iloc[val_idxs], targets.iloc[val_idxs]
        model, train_rmse, val_rmse = train_and_evaluate(X_train, train_targets, X_val,
        models.append(model)
        train_rmses.append(train_rmse)
        val_rmses.append(val_rmse)
    print('Train RMSE: {}, Validation RMSE: {}'.format(np.mean(train_rmses), np.mean(va
    return models
```

Since it may take a long time to perform 5-fold cross validation for each set of parameters we wish to try, we'll just pick a random 10% sample of the dataset as the validation set.

```
from sklearn.model_selection import train_test_split
```

```
X_train, X_val, train_targets, val_targets = train_test_split(X, targets, test_size=0.1
```

```
def test_params(**params):
    model = XGBRegressor(n_jobs=-1, random_state=42, **params)
```

```
    model.fit(X_train, train_targets)
    train_rmse = rmse(model.predict(X_train), train_targets)
    val_rmse = rmse(model.predict(X_val), val_targets)
    print('Train RMSE: {}, Validation RMSE: {}'.format(train_rmse, val_rmse))
```

n_estimators

The number of trees to be created. More trees = greater capacity of the model.

```
test_params(n_estimators=10)
```

```
Train RMSE: 2353.663414241198, Validation RMSE: 2356.229854163455
```

```
test_params(n_estimators=30)
```

```
Train RMSE: 1911.2460991462647, Validation RMSE: 1915.6472657649233
```

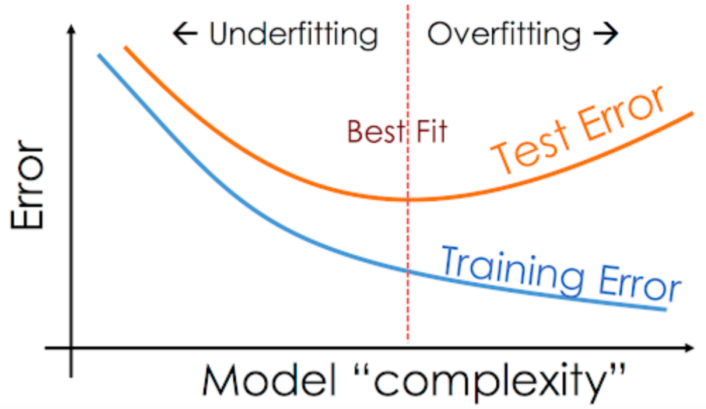
```
test_params(n_estimators=100)
```

```
Train RMSE: 1185.4562733444168, Validation RMSE: 1193.1959233994555
```

```
test_params(n_estimators=240)
```

```
Train RMSE: 895.8322715342299, Validation RMSE: 910.1409179651465
```

> **EXERCISE**: Experiment with different values of `n_estimators`, plot a graph of the training and validation error and determine the best value for `n_estimators`.




```

```

```

```

max_depth

As you increase the max depth of each tree, the capacity of the tree increases and it can capture more information about the training set.

```
test_params(max_depth=2)
```

```
Train RMSE: 2354.679896364511, Validation RMSE: 2351.1681023945134
```

```
test_params(max_depth=5)
```

```
Train RMSE: 1456.0644283203644, Validation RMSE: 1457.2885926259178
```

```
test_params(max_depth=10)
```

```
Train RMSE: 691.2025514846819, Validation RMSE: 777.7774318826166
```

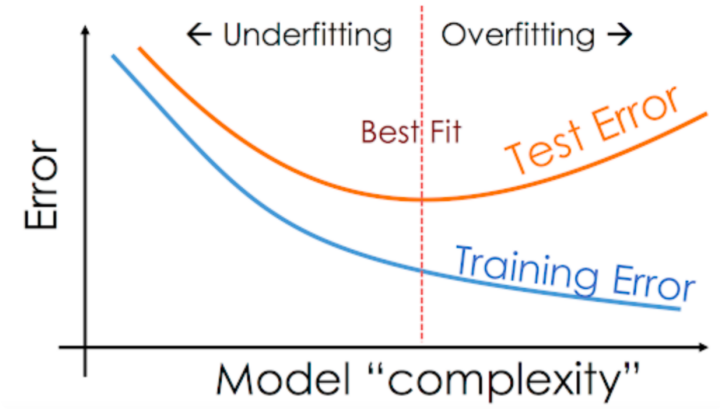
```

```

```

```

> **EXERCISE**: Experiment with different values of `max_depth` , plot a graph of the training and validation error and determine the optimal.



`learning_rate`

The scaling factor to be applied to the prediction of each tree. A very high learning rate (close to 1) will lead to overfitting, and a low learning rate (close to 0) will lead to underfitting.

```
test_params(n_estimators=50, learning_rate=0.01)
```

```
Train RMSE: 5044.000166628424, Validation RMSE: 5039.631093589314
```

```
test_params(n_estimators=50, learning_rate=0.1)
```

```
Train RMSE: 2167.858504538518, Validation RMSE: 2167.2963858379153
```

```
test_params(n_estimators=50, learning_rate=0.3)
```

```
Train RMSE: 1559.3736718929556, Validation RMSE: 1566.68780047217
```

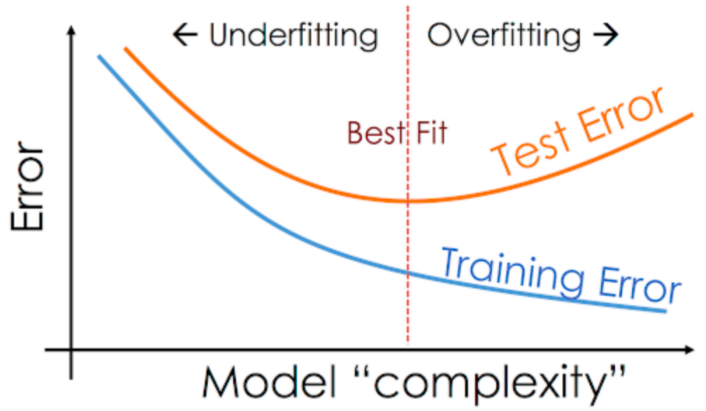
```
test_params(n_estimators=50, learning_rate=0.9)
```

```
Train RMSE: 1115.8929050462332, Validation RMSE: 1124.0787360992879
```

```
test_params(n_estimators=50, learning_rate=0.99)
```

```
Train RMSE: 1141.0686753930636, Validation RMSE: 1153.9657795546302
```

> **EXERCISE**: Experiment with different values of `learning_rate`, plot a graph of the training and validation error and determine the optimal.




```

```

```

```

booster

Instead of using Decision Trees, XGBoost can also train a linear model for each iteration. This can be configured using `booster`.

```
test_params(booster='gblinear')
```

```
Train RMSE: 217054.65872292817, Validation RMSE: 217077.36665393168
```

Clearly, a linear model is not well suited for this dataset.

> **EXERCISE**: Exeperiment with other hyperparameters like `gamma`, `min_child_weight`, `max_delta_step`, `subsample`, `colsample_bytree` etc. and find their optimal values. Learn more about them here: https://xgboost.readthedocs.io/en/latest/python/python_api.html#xgboost.XGBRegressor

```

```

> **EXERCISE**: Train a model with your best hyperparmeters and evaluate its peformance using 5-fold cross validation.

Let's save our work before continuing.

```
jovian.commit()
```

Putting it Together and Making Predictions

Let's train a final model on the entire training set with custom hyperparameters.

```
model = XGBRegressor(n_jobs=-1, random_state=42, n_estimators=1000,
                     learning_rate=0.2, max_depth=10, subsample=0.9,
                     colsample_bytree=0.7)
```

```
%%time
model.fit(X, targets)
```

```
CPU times: user 1h 25min 32s, sys: 1min 35s, total: 1h 27min 8s
Wall time: 5min 54s
```

```
XGBRegressor(base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=0.7, gamma=0, gpu_id=-1,
             importance_type='gain', interaction_constraints='',
             learning_rate=0.2, max_delta_step=0, max_depth=10,
             min_child_weight=1, missing=nan, monotone_constraints='()',
             n_estimators=1000, n_jobs=-1, num_parallel_tree=1, random_state=42,
             reg_alpha=0, reg_lambda=1, scale_pos_weight=1, subsample=0.9,
             tree_method='exact', validate_parameters=1, verbosity=None)
```

Now that the model is trained, we can make predictions on the test set.

```
test_preds = model.predict(X_test)
```

Let's add the predictions into `submission_df` .

```
submission_df['Sales']  = test_preds
```

Recall, however, if if the store is not open, then the sales must be 0. Thus, wherever the value of `Open` in the test set is 0, we can set the sales to 0. Also, there some missing values for `Open` in the test set. We'll replace them with 1 (open).

```
test_df.Open.isna().sum()
```

11

```
submission_df['Sales'] = submission_df['Sales'] * test_df.Open.fillna(1.)
```

```
submission_df
```

	Id	Sales
0	1	4207.074707
1	2	7587.398438
2	3	8849.461914
3	4	7390.013184
4	5	7085.753418
...	...	...
41083	41084	1868.461792
41084	41085	7354.468262
41085	41086	6223.554688
41086	41087	24107.359375
41087	41088	6790.744629

41088 rows × 2 columns

We can now save the predictions as a CSV file.

```
submission_df.to_csv('submission.csv', index=None)
```

```
from IPython.display import FileLink
```

```
# Doesn't work on Colab, use the file browser instead.
FileLink('submission.csv')
```

submission.csv

We can now make a submission on this page and check our score: https://www.kaggle.com/c/rossmann-store-sales/submit

> **EXERCISE**: Experiment with different models and hyperparameters and try to beat the above score. Take inspiration from the top notebooks on the "Code" tab of the competition.

```

```

```

```

> **EXERCISE**: Save the model and all the other required objects using `joblib`.

```

```

```

```

> **EXERCISE**: Write a function `predict_input` which can make predictions for a single input provided as a dictionary. Make sure to include all the feature engineering and preprocessing steps. Refer to previous tutorials for hints.

```

```

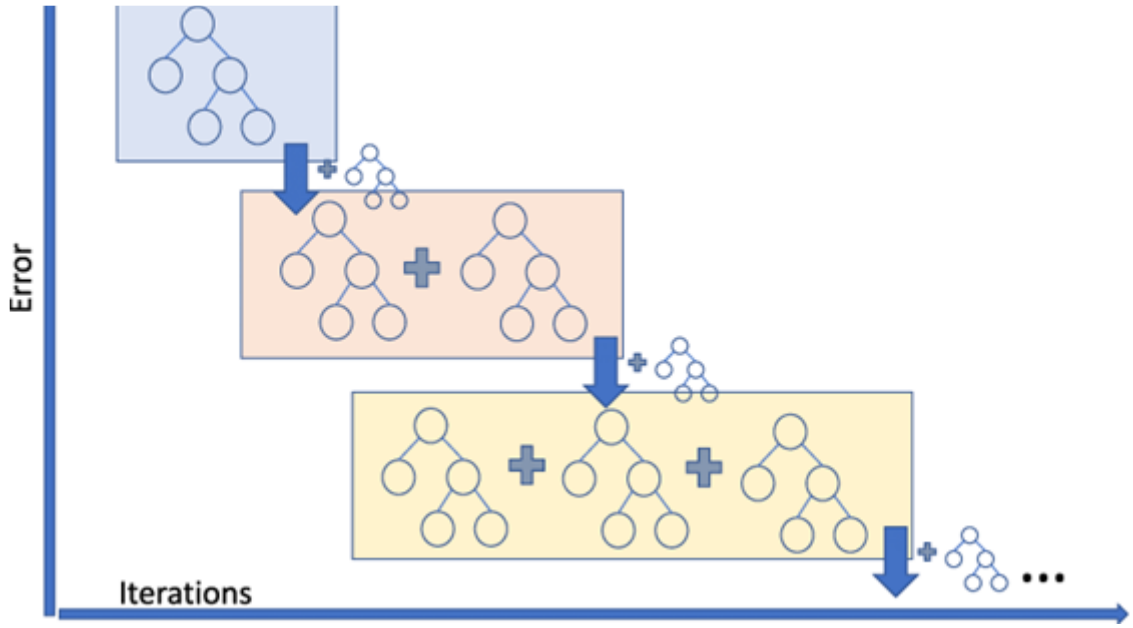
Let's save our work before continuing.

```
jovian.commit()
```

```
[jovian] Updating notebook "aakashns/python-gradient-boosting-machines" on https://jovian.ai/
[jovian] Committed successfully! https://jovian.ai/aakashns/python-gradient-boosting-machines
```

```
'https://jovian.ai/aakashns/python-gradient-boosting-machines'
```

Summary and References



The following topics were covered in this tutorial:

- Downloading a real-world dataset from a Kaggle competition
- Performing feature engineering and prepare the dataset for training
- Training and interpreting a gradient boosting model using XGBoost
- Training with KFold cross validation and ensembling results
- Configuring the gradient boosting model and tuning hyperparamters

Check out these resources to learn more:

- https://albertum.medium.com/l1-l2-regularization-in-xgboost-regression-7b2db08a59e0
- https://machinelearningmastery.com/evaluate-gradient-boosting-models-xgboost-python/
- https://xgboost.readthedocs.io/en/latest/python/python_api.html#xgboost.XGBRegressor
- https://xgboost.readthedocs.io/en/latest/parameter.html
- https://www.kaggle.com/xwxw2929/rossmann-sales-top1

Revision Questions

1. What is a Gradient Boosting Machine (GBM) model?
2. What does term 'gradient' refer to?
3. What does term 'boosting' refer to?
4. What are weights and bias?
5. How to choose differentiate/choose numerical and categorical columns?
6. Why do you scale numerical columns?
7. Why do you encode categorical columns?
8. What is rankdir in `plot_tree()`?
9. What is the working of K-fold cross validation?
10. How does gamma hyperparameter work?

11. What is generalization?
12. What is ensembling?
13. What are the different ways to impute missing data?
14. What are the advantages of XGBoost?
15. What are the disadvantages of XGBoost?
16. What are the data pre-processing steps for XGBoost?
17. What is `rcParams`?
18. What does `get_dump()` do?
19. What is the difference between XGBoost and LightGBM?
20. Is XGBoost faster than Random Forest? If so, why?