Predicting Concrete Compressive Strength From Its Components Quantities

Introduction

Concrete is the most important material in civil engineering and it is of five major elements in various proportions: cement, water, coarse aggregates, fine aggregates (i.e. sand), and air. Concrete admixtures are natural or manufactured chemicals or additives added during concrete mixing to enhance specific properties of the fresh or hardened concrete, such as workability, durability, or early and final strength. The concrete compressive strength is a function of age and ingredients. The have been several research to develop the optimum mixure of Concrete.

Problem Statement

The Concrete research usually uses Concrete Compressive Strength Test in lab to find out the resultant strengths of different combination of concrete ingredients. This can be costly and time consuming. In this project, I will predict the compressive strength of concrete mixure measured in MPa using the historical records of previous testing and regression analysis methods.

Data Source

This dataset was taken from UCI Repository

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Date Donated: August 3, 2007

The following table shows the names of the variables and their meanings

variable	meaning and measurement unit
cement	quantitative, kg in a m3 mixture, Input Variable
slag	Blast Furnace Slag, quantitative, kg in a m3 mixture,Input Variable
flyash	Fly Ash, quantitative, kg in a m3 mixture,Input Variable
water	Blast Furnace Slag, quantitative, kg in a m3 mixture,Input Variable
superplasticizer	Superplasticizer, quantitative, kg in a m3 mixture,Input Variable
coarseaggregate	Coarse Aggregate, quantitative, kg in a m3 mixture,Input Variable
fineaggregate	Fine Aggregate, quantitative, kg in a m3 mixture,Input Variable
age	Age quantitative, Day (1~365), Input Variable
csMPa	Concrete compressive strength, quantitative, MPa, Output Variable

Data Extraction & Preparation

In this section, I extract the data from a csv file, analyze it a little and prepare it for further analysis

```
import numpy
import pandas as pd
```

```
df = pd.read_csv('../data/Concrete_Data.csv')
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1030 entries, 0 to 1029
Data columns (total 9 columns):
 #   Column            Non-Null Count  Dtype
---  ------            --------------  -----
 0   cement            1030 non-null   float64
 1   slag              1030 non-null   float64
 2   flyash            1030 non-null   float64
 3   water             1030 non-null   float64
 4   superplasticizer  1030 non-null   float64
 5   coarseaggregate   1030 non-null   float64
 6   fineaggregate     1030 non-null   float64
 7   age               1030 non-null   int64
 8   csMPa             1030 non-null   float64
dtypes: float64(8), int64(1)
memory usage: 72.5 KB
```

```
df.rename(columns={'flyash':'flya_ash',
                   'superplasticizer':'super_plasticizer',
                   'coarseaggregate':'coarse_aggregate',
                   'fineaggregate':'fine_aggregate',
                   'csMPa':'compressive_strength_csMPa'
                  }, inplace=True)

df.head()
```

	cement	slag	flya_ash	water	super_plasticizer	coarse_aggregate	fine_aggregate	age	compressive_strength_csMPa
0	540.0	0.0	0.0	162.0	2.5	1040.0	676.0	28	79.99
1	540.0	0.0	0.0	162.0	2.5	1055.0	676.0	28	61.89
2	332.5	142.5	0.0	228.0	0.0	932.0	594.0	270	40.27
3	332.5	142.5	0.0	228.0	0.0	932.0	594.0	365	41.05
4	198.6	132.4	0.0	192.0	0.0	978.4	825.5	360	44.30

Checking for Missing Values in the Data

```
df.isnull().sum()
```

```
cement                       0
slag                         0
flya_ash                     0
water                        0
super_plasticizer            0
coarse_aggregate             0
fine_aggregate               0
age                          0
compressive_strength_csMPa   0
dtype: int64
```

Checking for Duplicates Rows

```
df[df.duplicated(keep = False)]
```

	cement	slag	flya_ash	water	super_plasticizer	coarse_aggregate	fine_aggregate	age	compressive_strength_csMPa
72	425.0	106.3	0.0	153.5	16.5	852.1	887.1	3	33.40
77	425.0	106.3	0.0	153.5	16.5	852.1	887.1	3	33.40
80	425.0	106.3	0.0	153.5	16.5	852.1	887.1	3	33.40
83	362.6	189.0	0.0	164.9	11.6	944.7	755.8	3	35.30
86	362.6	189.0	0.0	164.9	11.6	944.7	755.8	3	35.30
88	362.6	189.0	0.0	164.9	11.6	944.7	755.8	3	35.30
91	362.6	189.0	0.0	164.9	11.6	944.7	755.8	3	35.30
95	425.0	106.3	0.0	153.5	16.5	852.1	887.1	7	49.20
100	425.0	106.3	0.0	153.5	16.5	852.1	887.1	7	49.20
103	425.0	106.3	0.0	153.5	16.5	852.1	887.1	7	49.20
106	362.6	189.0	0.0	164.9	11.6	944.7	755.8	7	55.90
109	362.6	189.0	0.0	164.9	11.6	944.7	755.8	7	55.90
111	362.6	189.0	0.0	164.9	11.6	944.7	755.8	7	55.90
118	425.0	106.3	0.0	153.5	16.5	852.1	887.1	28	60.29
123	425.0	106.3	0.0	153.5	16.5	852.1	887.1	28	60.29
126	425.0	106.3	0.0	153.5	16.5	852.1	887.1	28	60.29
129	362.6	189.0	0.0	164.9	11.6	944.7	755.8	28	71.30
132	362.6	189.0	0.0	164.9	11.6	944.7	755.8	28	71.30
134	362.6	189.0	0.0	164.9	11.6	944.7	755.8	28	71.30
137	362.6	189.0	0.0	164.9	11.6	944.7	755.8	28	71.30
141	425.0	106.3	0.0	153.5	16.5	852.1	887.1	56	64.30
146	425.0	106.3	0.0	153.5	16.5	852.1	887.1	56	64.30
149	425.0	106.3	0.0	153.5	16.5	852.1	887.1	56	64.30
152	362.6	189.0	0.0	164.9	11.6	944.7	755.8	56	77.30
155	362.6	189.0	0.0	164.9	11.6	944.7	755.8	56	77.30
157	362.6	189.0	0.0	164.9	11.6	944.7	755.8	56	77.30
160	362.6	189.0	0.0	164.9	11.6	944.7	755.8	56	77.30
164	425.0	106.3	0.0	153.5	16.5	852.1	887.1	91	65.20
169	425.0	106.3	0.0	153.5	16.5	852.1	887.1	91	65.20
172	425.0	106.3	0.0	153.5	16.5	852.1	887.1	91	65.20
175	362.6	189.0	0.0	164.9	11.6	944.7	755.8	91	79.30
177	362.6	189.0	0.0	164.9	11.6	944.7	755.8	91	79.30
179	362.6	189.0	0.0	164.9	11.6	944.7	755.8	91	79.30

182	362.6	189.0	0.0	164.9	11.6	944.7	755.8	91	79.30
801	252.0	0.0	0.0	185.0	0.0	1111.0	784.0	28	19.69
809	252.0	0.0	0.0	185.0	0.0	1111.0	784.0	28	19.69

Interesting!

It seems that some records are entered more than once. This may affect the results of the analysis!

I will keep the first record and remove its duplicate.

Droping the Duplicate rows

```
df.drop_duplicates(keep='first', inplace=True)
```

Now, data is ready for further analysis

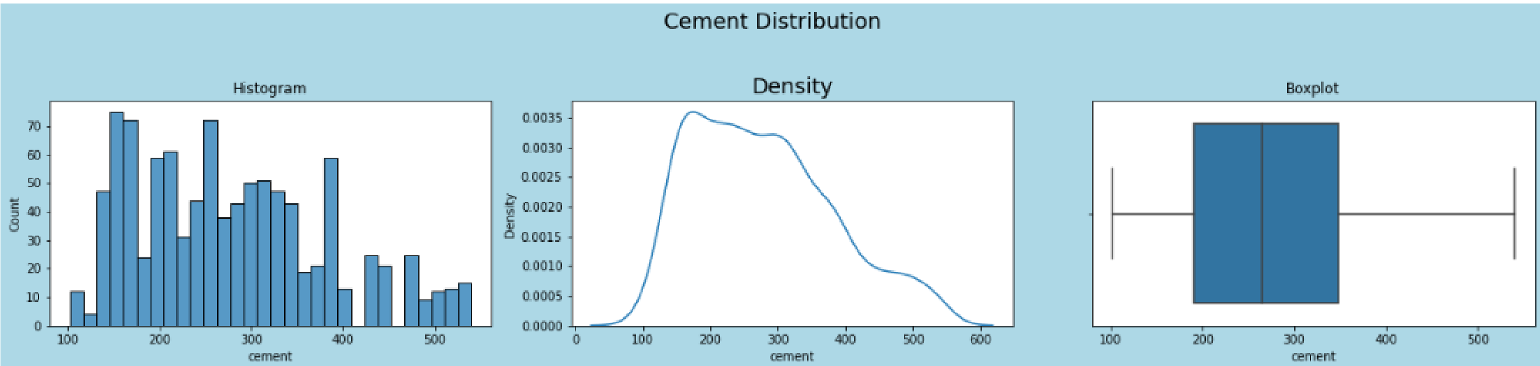
Exploratory Data Analysis

```
import matplotlib.pyplot as plt
import seaborn as sns
from scipy.stats.mstats import normaltest
```

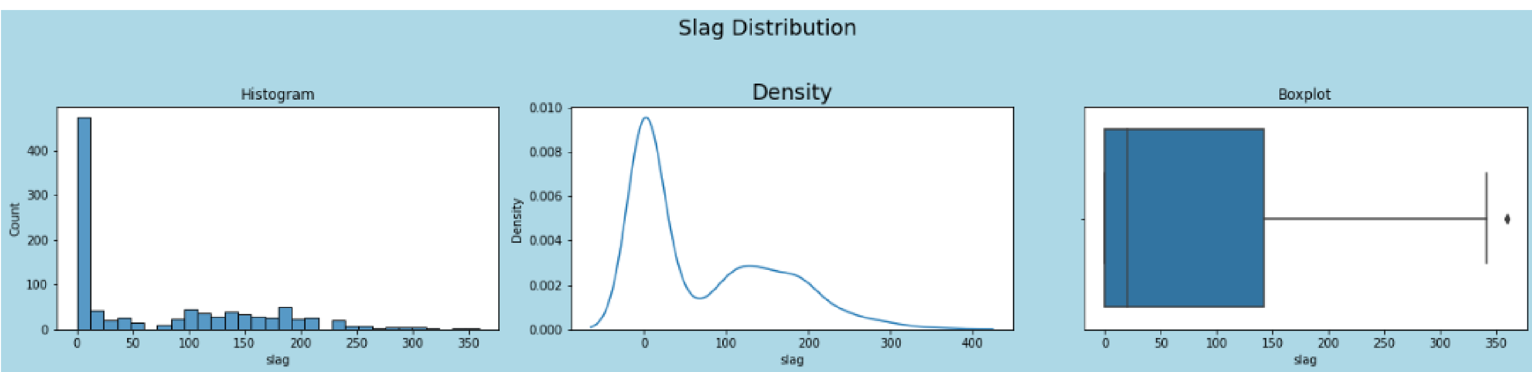
Checking The Distributions of the Variables (features nd target)

```
for col in df.columns.tolist():
    print(f'{col.capitalize()}')
    print(f'{col.capitalize()} Statistics')
    print(df[col].describe())
    print('\n')


    _, pvalue = normaltest(df[col].values)
    if pvalue < 0.05:
        result = f'{col} not normally distributed'
    else:
        result = f'{col} normally distributed'
    print(f'{col.capitalize()} Normality Test Result')
    print('P-value:',str(pvalue),',    Decision: ',result)


    plt.figure(figsize=(18,4), facecolor='lightblue')
    plt.suptitle(f'{col.capitalize()} Distribution',size = 18, y = 1.05)

    plt.subplot(1,3,1)
    sns.histplot(data=df, x = col, bins=30)
    plt.title('Histogram')

    plt.subplot(1,3,2)
    plt.title('Density', size = 18)
    sns.kdeplot(data=df[col])

    plt.subplot(1,3,3)
    sns.boxplot(data=df, x = col)
    plt.title('Boxplot')


    plt.tight_layout()
    plt.show()
```

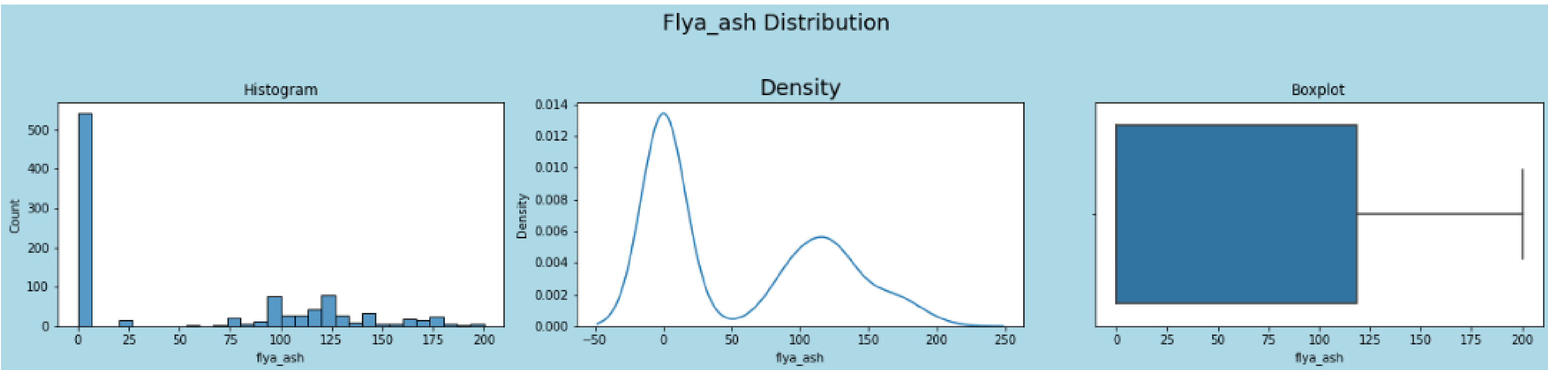
```
Cement
Cement Statistics
count    1005.000000
mean      278.631343
std       104.344261
min       102.000000
25%       190.700000
50%       265.000000
75%       349.000000
max       540.000000
Name: cement, dtype: float64


Cement Normality Test Result
P-value: 9.809278312609514e-14 ,    Decision:  cement not normally distributed
```



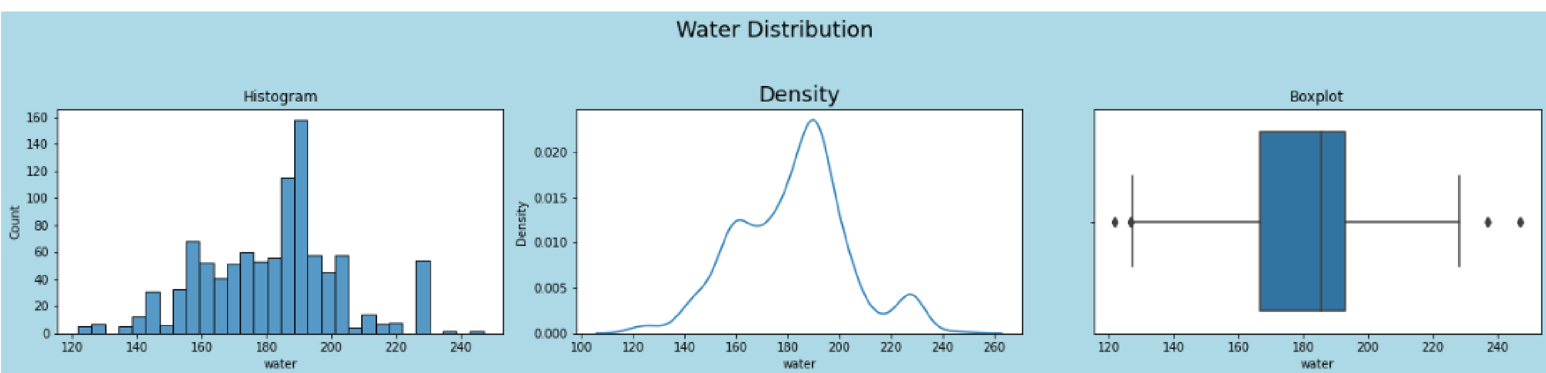

```
Slag
Slag Statistics
count    1005.000000
mean       72.043483
std        86.170807
min         0.000000
25%         0.000000
50%        20.000000
75%       142.500000
max       359.400000
Name: slag, dtype: float64


Slag Normality Test Result
P-value: 1.0885008864076576e-23 ,    Decision:  slag not normally distributed
```



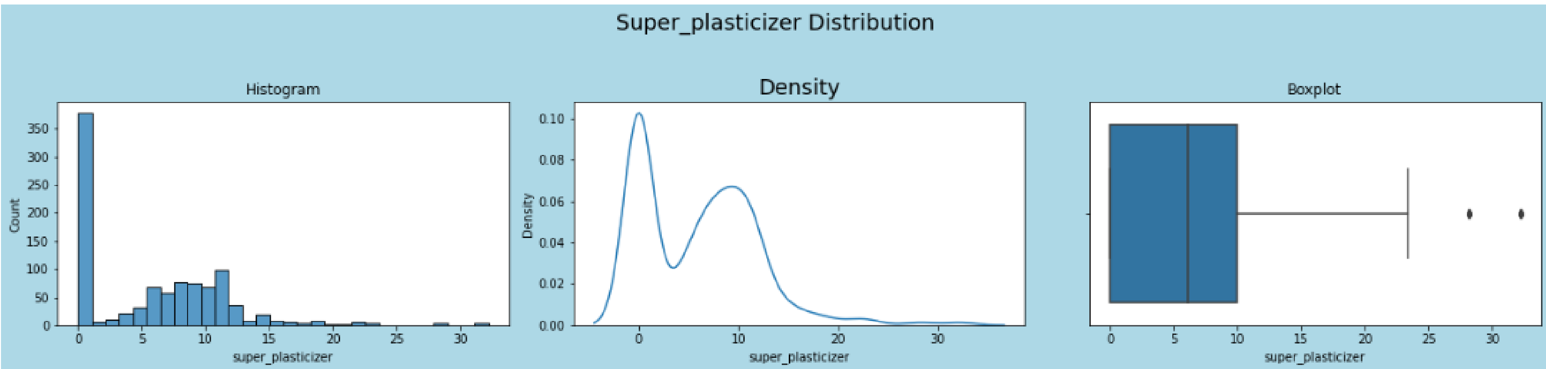
```
Flya_ash
Flya_ash Statistics
count    1005.000000
mean       55.536318
std        64.207969
min         0.000000
25%         0.000000
50%         0.000000
75%       118.300000
max       200.100000
Name: flya_ash, dtype: float64


Flya_ash Normality Test Result
P-value: 0.0 ,    Decision:  flya_ash not normally distributed
```



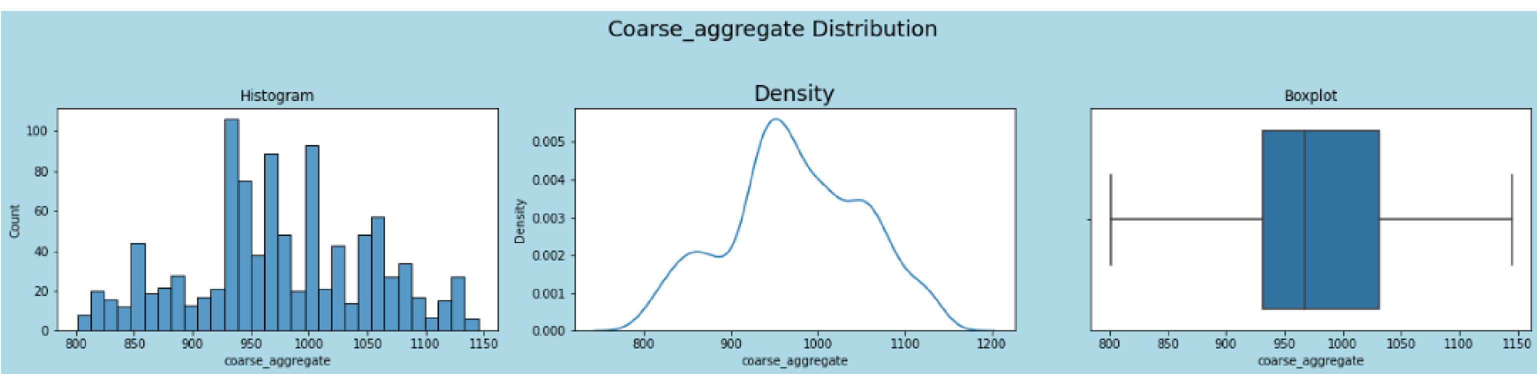

```
Water
Water Statistics
count    1005.000000
mean      182.075323
std        21.339334
min       121.800000
25%       166.600000
50%       185.700000
75%       192.900000
max       247.000000
Name: water, dtype: float64


Water Normality Test Result
P-value: 0.5005793792135014 ,    Decision:  water normally distributed
```



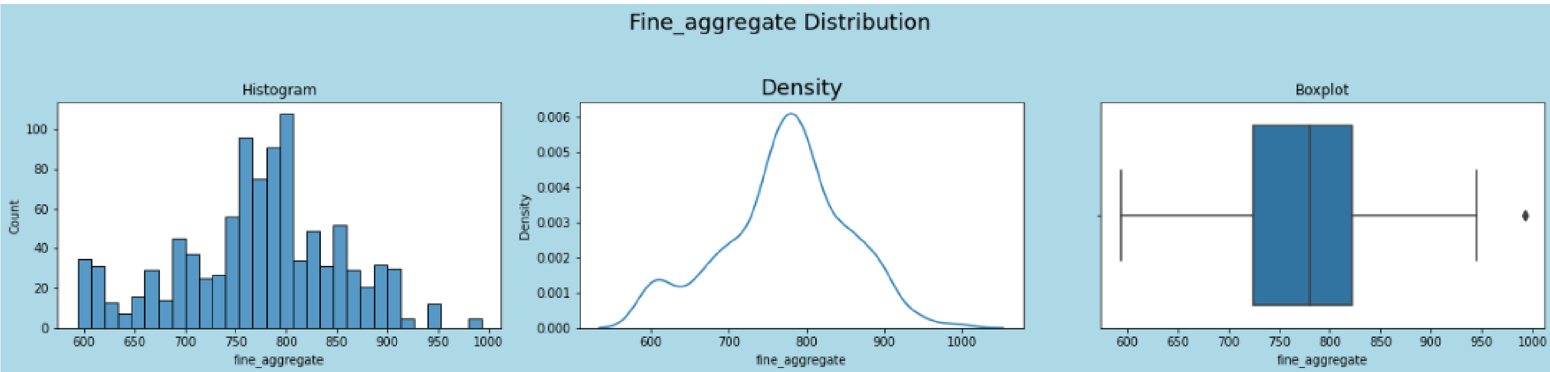
```
Super_plasticizer
Super_plasticizer Statistics
count    1005.000000
mean        6.033234
std         5.919967
min         0.000000
25%         0.000000
50%         6.100000
75%        10.000000
max        32.200000
Name: super_plasticizer, dtype: float64


Super_plasticizer Normality Test Result
P-value: 3.9839459643086454e-35 ,    Decision:  super_plasticizer not normally distributed
```



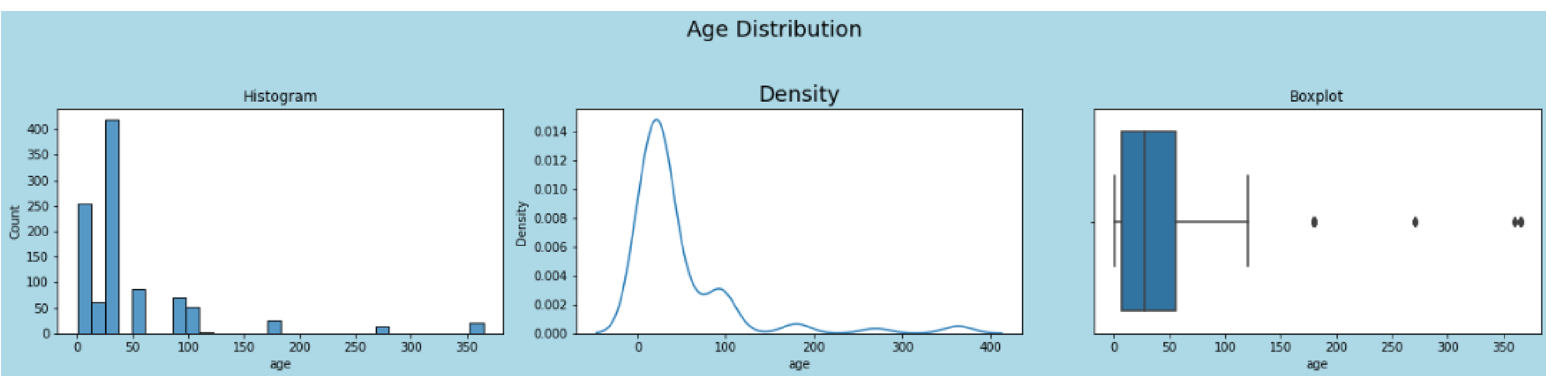

```
Coarse_aggregate
Coarse_aggregate Statistics
count    1005.000000
mean      974.376816
std        77.579667
min       801.000000
25%       932.000000
50%       968.000000
75%      1031.000000
max      1145.000000
Name: coarse_aggregate, dtype: float64


Coarse_aggregate Normality Test Result
P-value: 3.448426277401913e-07 ,    Decision:  coarse_aggregate not normally distributed
```



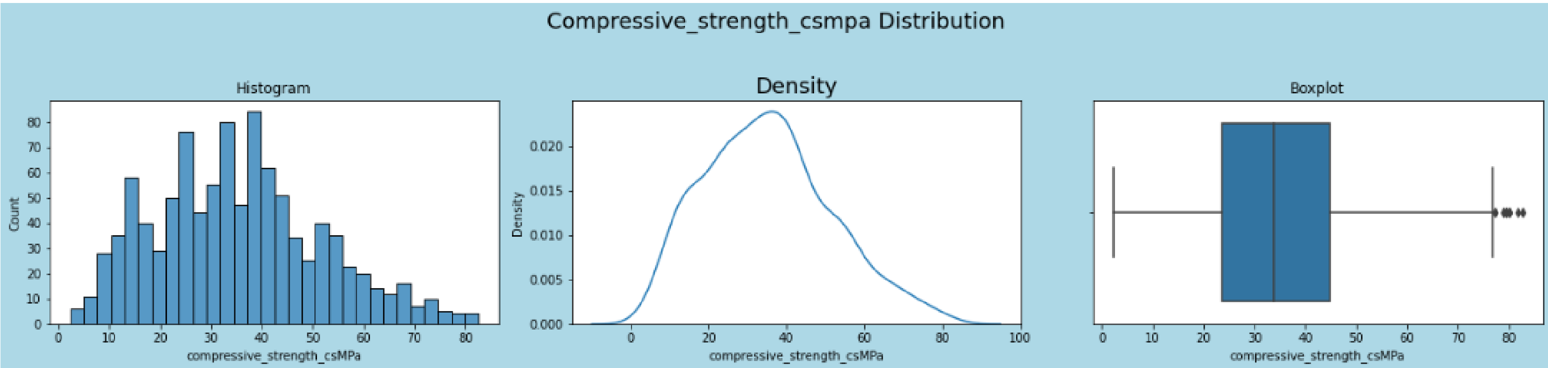
```
Fine_aggregate
Fine_aggregate Statistics
count    1005.000000
mean      772.688259
std        80.340435
min       594.000000
25%       724.300000
50%       780.000000
75%       822.200000
max       992.600000
Name: fine_aggregate, dtype: float64


Fine_aggregate Normality Test Result
P-value: 0.004291006583264156 ,    Decision:  fine_aggregate not normally distributed
```




```
Age
Age Statistics
count    1005.000000
mean       45.856716
std        63.734692
min         1.000000
25%         7.000000
50%        28.000000
75%        56.000000
max       365.000000
Name: age, dtype: float64


Age Normality Test Result
P-value: 3.9929469938994235e-154 ,    Decision:  age not normally distributed
```



```
Compressive_strength_csmpa
Compressive_strength_csmpa Statistics
count    1005.000000
mean       35.250378
std        16.284815
min         2.330000
25%        23.520000
50%        33.800000
75%        44.870000
max        82.600000
Name: compressive_strength_csMPa, dtype: float64


Compressive_strength_csmpa Normality Test Result
P-value: 3.154432677195138e-07 ,    Decision:  compressive_strength_csMPa not normally distributed
```



Features Non-normality

Some beginners think (erroneously) that the normal distribution assumption of linear regression applies to their data. They might plot their response variable as a histogram and examine whether it differs from a normal distribution. Others assume that the explanatory variable must be normally-distributed. Neither is required. The normality assumption relates to the distributions of the residuals. This is assumed to be normally distributed, and the regression line is fitted to the data such that the mean of the residuals is zero.
Source

Removing Outliers From Target

It can be seen that the target contains some outliers. Removing those outliers can imporove the scoring of the model. There are two methods for detecting and removing outliers. For normally distributed data I can use (mean - 3*standard_deviation) and (mean* + 3standard_deviation). For non normally distibuted data, I can use the interquartile method.Since the data is not normally distributed, I will use the interquartile method

```
q1 = df.compressive_strength_csMPa.quantile(0.25)
q3 = df.compressive_strength_csMPa.quantile(0.75)
iqr = q3-q1
upper_lim = q3 + 1.5*iqr
lower_lim = q1 - 1.5*iqr

df = df[(df.compressive_strength_csMPa >= lower_lim) & (df.compressive_strength_csMPa <= upper_lim)]
```

Features Selection (based on statiscal testing)

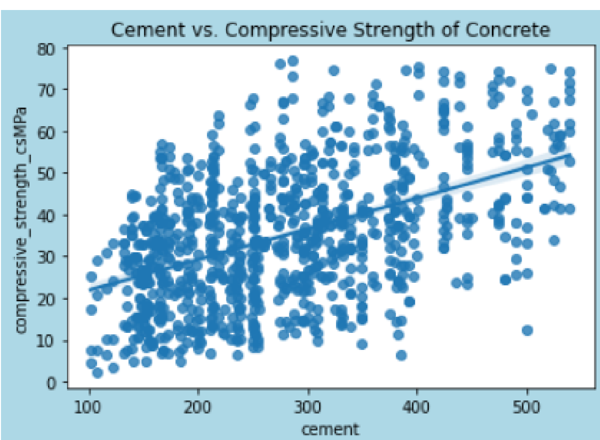
```
from scipy.stats import pearsonr
```

```
features = [col for col in df.columns if col != 'compressive_strength_csMPa']
y = df['compressive_strength_csMPa']

y.head()
```

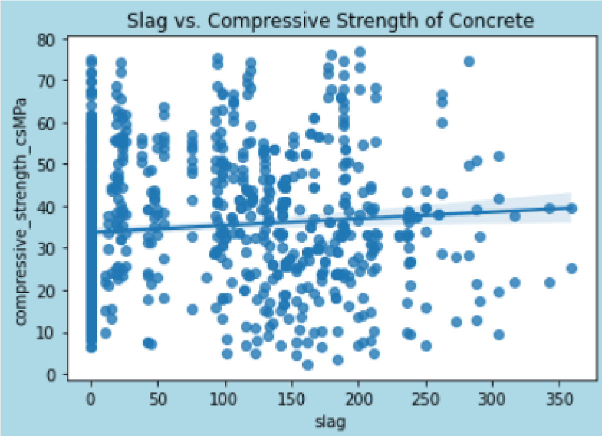
```
1    61.89
2    40.27
3    41.05
4    44.30
5    47.03
Name: compressive_strength_csMPa, dtype: float64
```

```
significant_features = []
for col in features:
    corr, p_value = pearsonr(df[col],df['compressive_strength_csMPa'])
    print(f'{col} vs. compressive_strength_csMPa:\n')
    print('Correlation Coefficient:',corr)
    print('p_value:',p_value)

    if p_value < 0.05:
        significant_features.append(col)
        if corr > 0:
            print(f'There is a significant evidence of a positive relationship between {col} and Concrete Compressive Strength')
        else:
            print(f'There is a significant evidence of a negative relationship between {col} and Concrete Compressive Strength')
    else:
        print(f'There is no significant relationship between {col} and Concrete Compressive Strength')

    plt.figure(figsize = (6,4), facecolor='lightblue')
    plt.title(f'{col.capitalize()} vs. Compressive Strength of Concrete')
    sns.regplot(x=col, y='compressive_strength_csMPa',data=df)
    plt.show()
```

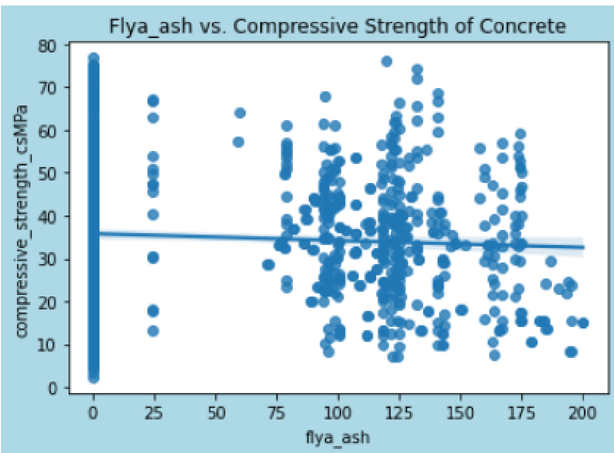
```
cement vs. compressive_strength_csMPa:

Correlation Coefficient: 0.4822980854149247
p_value: 3.260615343299635e-59
There is a significant evidence of a positive relationship between cement and Concrete Compressive Strength
```



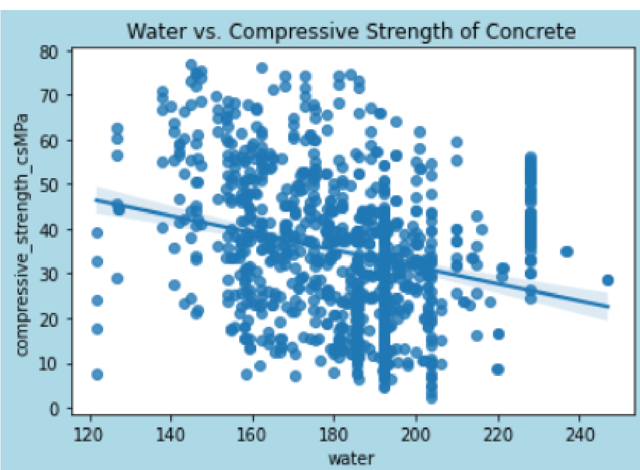
```
Correlation Coefficient: 0.08746360483548354
p_value: 0.0057181044887169895
There is a significant evidence of a positive relationship between slag and Concrete Compressive Strength
```



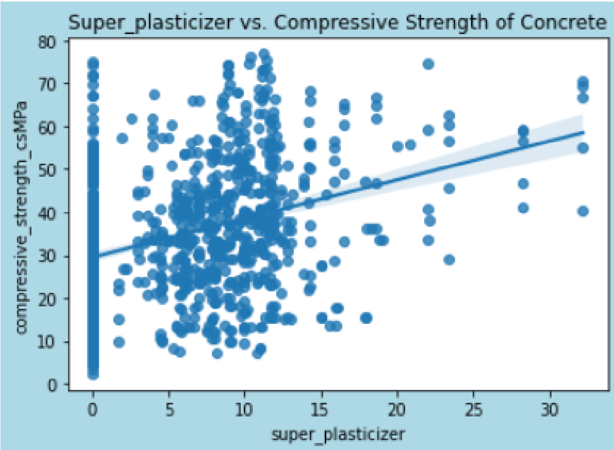

```
Correlation Coefficient: -0.06373667178654671
p_value: 0.04421716444068777
There is a significant evidence of a negative relationship between flya_ash and Concrete Compressive Strength
```



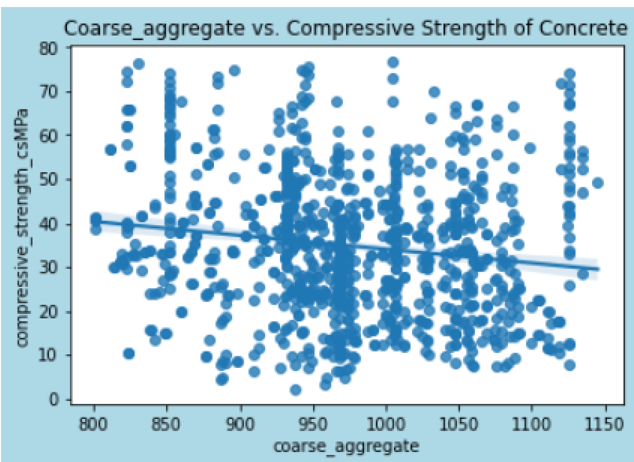

```
Correlation Coefficient: -0.2555851420974356
p_value: 2.473472671917299e-16
There is a significant evidence of a negative relationship between water and Concrete Compressive Strength
```



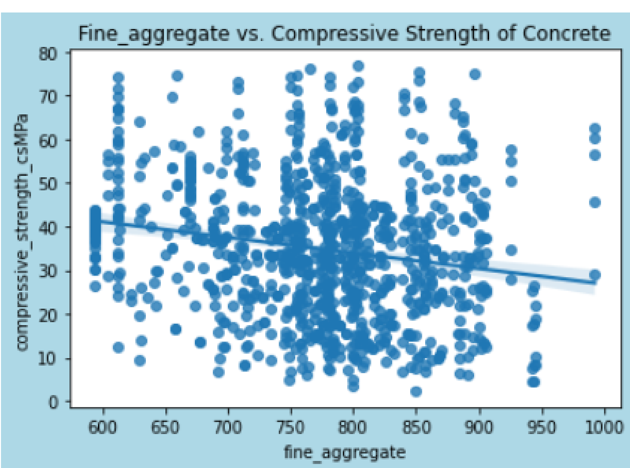
```
Correlation Coefficient: 0.33453422476340167
p_value: 1.704786278505969e-27
There is a significant evidence of a positive relationship between super_plasticizer and Concrete Compressive Strength
```



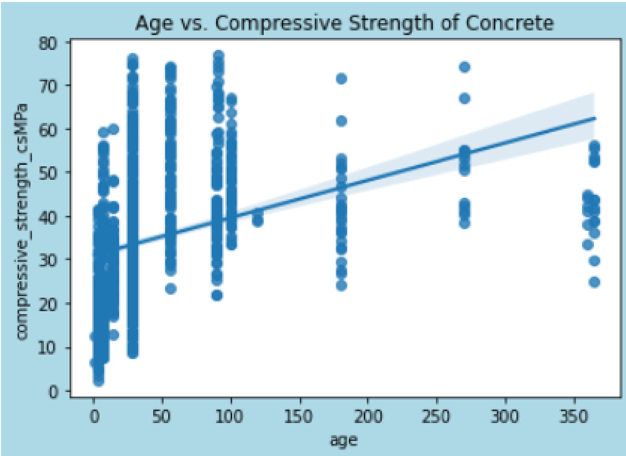

```
Correlation Coefficient: -0.15460377731918934
p_value: 9.339984407882778e-07
There is a significant evidence of a negative relationship between coarse_aggregate and Concrete Compressive Strength
```




```
Correlation Coefficient: -0.18091803888531244
p_value: 8.771870787097434e-09
There is a significant evidence of a negative relationship between fine_aggregate and Concrete Compressive Strength
```



```
Correlation Coefficient: 0.34524351184373747
p_value: 2.752890440217549e-29
There is a significant evidence of a positive relationship between age and Concrete Compressive Strength
```



Dividing the Data to Features (X) and Target (y)

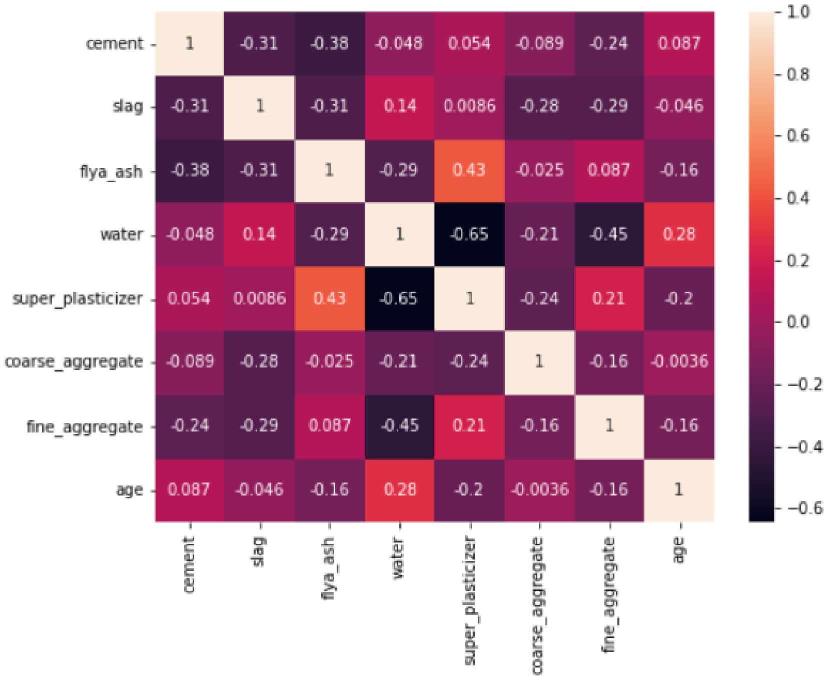
```
X_initial = df[significant_features]

print(X_initial.head())
```

```
   cement   slag  flya_ash  water  super_plasticizer  coarse_aggregate  \
1   540.0    0.0       0.0  162.0                2.5            1055.0
2   332.5  142.5       0.0  228.0                0.0             932.0
3   332.5  142.5       0.0  228.0                0.0             932.0
4   198.6  132.4       0.0  192.0                0.0             978.4
5   266.0  114.0       0.0  228.0                0.0             932.0

   fine_aggregate  age
1           676.0   28
2           594.0  270
3           594.0  365
4           825.5  360
5           670.0   90
```

Checking for Mutlicollinearity

As a graduate of Civil Engineering (domain knowledge), I knwo there is no multicollinearity between the components of concrete mixutres as each material or addtive serves different function. However, as machine learnign best practice, I should check for multicollinearity

```python
corr = X_initial.corr()
plt.figure(figsize=(8,6))
sns.heatmap(corr, annot=True)
plt.xticks();
```



Looking at the values of pearson correlation, there is no significant maulticollinearity!

Feature Egineering

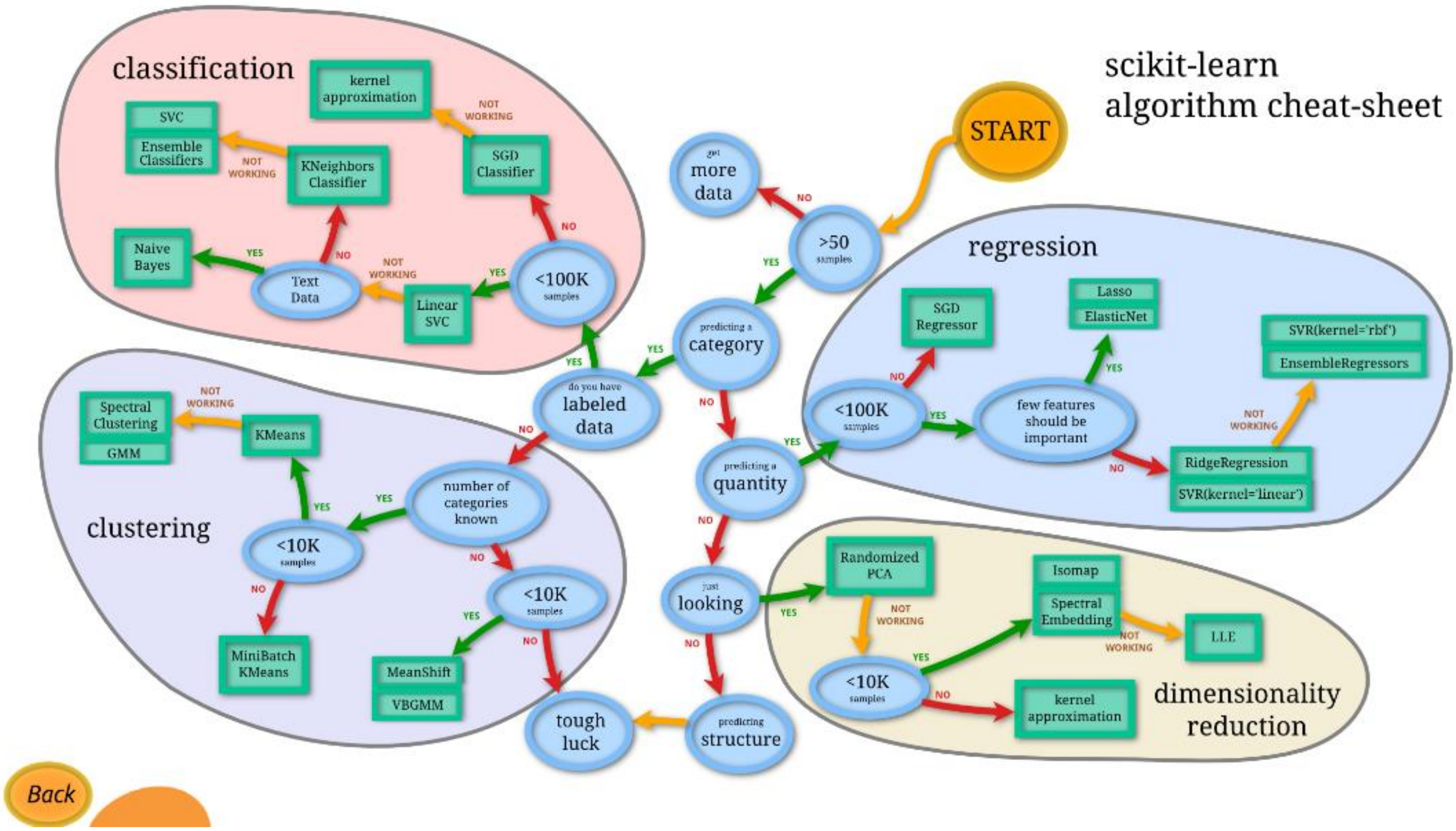
```python
from sklearn.preprocessing import StandardScaler

from sklearn.model_selection import train_test_split
```

Scaling the Features

```python
# It is essential for the featurs of a regression models to on the same scale

standarizing_transformer = StandardScaler()

X_scaled = standarizing_transformer.fit_transform(X_initial)

X_scaled = pd.DataFrame(X_scaled, columns = X_initial.columns)


# Although it is not necessary to normalize the targte varibale, sometimes it may lead to
# better model.
y = numpy.log1p(y)
```

```python
# divide the data into train and test datasets
X_train, X_test, y_train, y_test = train_test_split(X_scaled, y,
                                                    test_size = 0.2, random_state = 2)
```

Model Selection and Evaluation



Strategy

Selecting an Estimator

- I will take the recommendation of sklearn documentation with some modification.
- I will test several baseline models initially.
- Next, I will try several ensemble regressors.
- Next, I will compares the performances of different baseline models.
- Finally, I will optimize and tune the selected model using GridSerachCV

Selecting Evaluation Scoring Metrics

I will use r2 since I don't know the permissible limit of error. The permissible limit of error differs depending on the objective of the study

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

from sklearn.linear_model import LinearRegression
from sklearn.linear_model import LinearRegression
from sklearn.linear_model import Ridge
from sklearn.linear_model import Lasso

from sklearn.svm import LinearSVR

from sklearn.neighbors import KNeighborsRegressor

from sklearn.tree import DecisionTreeRegressor

from sklearn.ensemble import AdaBoostRegressor,BaggingRegressor,GradientBoostingRegressor,RandomForestRegressor

from xgboost import XGBRegressor
```

Models Building

```
l_r = LinearRegression(n_jobs=-1)

r_r = Ridge(random_state = 2)

knn_r = KNeighborsRegressor(n_jobs=-1)

dt_r = DecisionTreeRegressor(random_state = 2)

rf_r = RandomForestRegressor(random_state = 2, n_jobs= -1)

bg_r = BaggingRegressor(random_state= 2, n_jobs=-1)

xgb_r = XGBRegressor(random_state= 2, n_jobs=-1)

ada_r = AdaBoostRegressor()

gb_r = GradientBoostingRegressor()


models = [('LinearRegression',l_r),
          ('Ridge',r_r),
          ('KNeighborsRegressor',knn_r),
          ('DecisionTreeRegressor',dt_r),
          ('RandomForestRegressor',rf_r),
          ('BaggingRegressor',bg_r),
          ('AdaBoostRegressor',ada_r),
          ('GradientBoostingRegressor',gb_r),
          ('XGBRegressor',xgb_r)
        ]


results = {'model': [],
           'r2_score':[],
           'mean_absolute_error':[]
          }
```

```
for model_name,  model in models:
    # X_transformed = polynomiallyTrasnformed_standarized_labeled(X,i)

    reg_model = model

    kf = KFold(n_splits=5, shuffle= True, random_state= 2).split(X_train,y_train)
    r2_scores =cross_val_score(reg_model, X_train,y_train,cv=kf, scoring='r2')

    kf = KFold(n_splits=5, shuffle= True, random_state= 2).split(X_train,y_train)
    mae_scores =cross_val_score(reg_model, X_train,y_train,cv=kf, scoring='neg_mean_absolute_error')


    results['model'].append(model_name)
    results['r2_score'].append(r2_scores.mean())
    results['mean_absolute_error'].append(-1*mae_scores.mean())

results_df = pd.DataFrame(results)
results_df = results_df.sort_values('r2_score', ascending=False).reset_index(drop=True)
results_df
```

	model	r2_score	mean_absolute_error
0	XGBRegressor	0.914634	0.096989
1	GradientBoostingRegressor	0.904129	0.115305
2	RandomForestRegressor	0.891026	0.118985
3	BaggingRegressor	0.870394	0.129581
4	AdaBoostRegressor	0.788531	0.190277
5	DecisionTreeRegressor	0.779214	0.157721
6	KNeighborsRegressor	0.648805	0.231035
7	Ridge	0.520315	0.282283
8	LinearRegression	0.519966	0.282256

So, the model with the best r2 scoring is XGBRegressor and with no ploynomial transofrmation

---

Testing the Selected Model

```
from sklearn.metrics import r2_score
```

```
model = XGBRegressor(random_state= 2, n_jobs=-1)

model.fit(X_train,y_train)

y_pred = model.predict(X_test)

print('The score of the test:')
print(r2_score(y_test,y_pred))
```

```
The score of the test:
0.9307441376190104
```

Tuning the Model

```
from sklearn.model_selection import GridSearchCV
```

```
xgb_r = XGBRegressor(random_state= 2, n_jobs=-1)

params_grid = {'eta':[0.1,0.2,0.3,0.4]}

kf = KFold(n_splits=5, shuffle= True, random_state= 2).split(X_scaled,y)

gs_xgb_r = GridSearchCV(xgb_r, params_grid, n_jobs=-1, cv = kf, scoring='r2')


gs_xgb_r.fit(X_scaled,y);

print('Best eta')
print(gs_xgb_r.best_params_)
print('\n')
print('Best score:')
print(gs_xgb_r.best_score_)
```

```
Best eta
{'eta': 0.2}


Best score:
0.9334140397687536
```

Model Interpretation

```
xgb_reg =  XGBRegressor(random_state= 2, n_jobs=-1, eta = 0.2)
xgb_reg.fit(X_scaled,y)


importance_df = pd.DataFrame({'feature':X_scaled.columns.to_list(),
                              'importance':xgb_reg.feature_importances_}).\
                                sort_values('importance',ascending=False)

importance_df
```

	feature	importance
7	age	0.312057
0	cement	0.204868
4	super_plasticizer	0.182134
1	slag	0.106332
3	water	0.074790
6	fine_aggregate	0.052398
2	flya_ash	0.037724
5	coarse_aggregate	0.029698

From the importance dataframe, it can be seen that the 3 most impactfull measureable factors in the compressive strength of the concrete are age (in days), cement amount and superplasticizer amount. For each 1 day, 1 unit of cement (kg in m3) and unit of superplasticizer (kg in m3) the compressive strength of ocncrete inscreases by 0.31 MPa, 0.2 MPa and 0.18 MPa respectively.

Saving the Model

```
import joblib
```

```
joblib.dump(xgb_reg, 'xgb_reg.pkl')
```

```
['xgb_reg.pkl']
```

This model can be used to estimate the compressive strength of concrete before carrying out the physical experiemnt. By experimenting with different values of (water, cement, fine aggregate...ect), a reseacher can use this model to estimate the corresponding concrete compressive strength before carrying out the actual experiment in the lab. That can save effort, time and cost.