Context

Concrete is the most important material in civil engineering. The concrete compressive strength is a highly nonlinear function of age and ingredients. These ingredients include cement, blast furnace slag, fly ash, water, superplasticizer, coarse aggregate, and fine aggregate.

Content

Data Characteristics:

The actual concrete compressive strength (MPa) for a given mixture under a specific age (days) was determined from laboratory. Data is in raw form (not scaled).

Summary Statistics:

Number of instances (observations): 1030

Number of Attributes: 9 Attribute breakdown: 8 quantitative input variables, and 1 quantitative output variable

Missing Attribute Values: None

Variable Information:

Given is the variable name, variable type, the measurement unit and a brief description. The concrete compressive strength is the regression problem. The order of this listing corresponds to the order of numerals along the rows of the database.

Name -- Data Type -- Measurement -- Description

Cement (component 1) -- quantitative -- kg in a m3 mixture -- Input Variable

Blast Furnace Slag (component 2) -- quantitative -- kg in a m3 mixture -- Input Variable

Fly Ash (component 3) -- quantitative -- kg in a m3 mixture -- Input Variable

Water (component 4) -- quantitative -- kg in a m3 mixture -- Input Variable

Superplasticizer (component 5) -- quantitative -- kg in a m3 mixture -- Input Variable

Coarse Aggregate (component 6) -- quantitative -- kg in a m3 mixture -- Input Variable

Fine Aggregate (component 7) -- quantitative -- kg in a m3 mixture -- Input Variable

Age -- quantitative -- Day (1~365) -- Input Variable

Concrete compressive strength -- quantitative -- MPa -- Output Variable

In [16]:

```
# Import data from kaggle
from google.colab import files
files.upload()                      # Upload kaggle.json file
! mkdir ~/.kaggle
! cp kaggle.json ~/.kaggle/
! chmod 600 ~/.kaggle/kaggle.json
! kaggle datasets download -d niteshyadav3103/concrete-compressive-strength
! unzip concrete-compressive-strength.zip
```

Choose File **No file selected**

Upload widget is only available when the cell has been executed in the current browser session. Please rerun this cell to enable.

```
Saving kaggle.json to kaggle (1).json
mkdir: cannot create directory '/root/.kaggle': File exists
concrete-compressive-strength.zip: Skipping, found more recently modified local copy (use
--force to force download)
Archive:  concrete-compressive-strength.zip
replace Concrete Compressive Strength.csv? [y]es, [n]o, [A]ll, [N]one, [r]ename: n
```

In [17]:

```python
# Modules
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
import warnings
warnings.simplefilter(action='ignore', category=FutureWarning)
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.model_selection import train_test_split, cross_val_score
from sklearn.linear_model import LinearRegression
from sklearn.tree import DecisionTreeRegressor
from sklearn.metrics import mean_absolute_error, mean_squared_error, r2_score
from sklearn.ensemble import RandomForestRegressor, GradientBoostingRegressor
from sklearn.neighbors import KNeighborsRegressor
from sklearn import svm
from sklearn.feature_selection import SelectKBest, f_regression
from xgboost import XGBRegressor
```

In [18]:

```python
# A look at the data
df = pd.read_csv('/content/Concrete Compressive Strength.csv')
df.head()
```

Out[18]:

	Cement (component 1)(kg in a m^3 mixture)	Blast Furnace Slag (component 2) (kg in a m^3 mixture)	Fly Ash (component 3)(kg in a m^3 mixture)	Water (component 4)(kg in a m^3 mixture)	Superplasticizer (component 5) (kg in a m^3 mixture)	Coarse Aggregate (component 6)(kg in a m^3 mixture)	Fine Aggregate (component 7)(kg in a m^3 mixture)	Age (day)	Concrete compressive strength(MPa, megapascals)
0	540.0	0.0	0.0	162.0	2.5	1040.0	676.0	28	79.986111
1	540.0	0.0	0.0	162.0	2.5	1055.0	676.0	28	61.887366
2	332.5	142.5	0.0	228.0	0.0	932.0	594.0	270	40.269535
3	332.5	142.5	0.0	228.0	0.0	932.0	594.0	365	41.052780
4	198.6	132.4	0.0	192.0	0.0	978.4	825.5	360	44.296075

As can be seen here, the column names contain a lot of information that is unnecessary for the analysis. Thus, this extra information is removed.

In [19]:

```python
# Remove extra information from column names
cols = df.columns
new_cols = []
for col in cols:
  col = col.split('(')[0].rstrip().lower().replace(' ','_')
  new_cols.append(col)
df.columns = new_cols
df.head()
```

Out[19]:

	cement	blast_furnace_slag	fly_ash	water	superplasticizer	coarse_aggregate	fine_aggregate	age	concrete_compressive_
0	540.0	0.0	0.0	162.0	2.5	1040.0	676.0	28	7

	cement	blast_furnace_slag	fly_ash	water	superplasticizer	coarse_aggregate	fine_aggregate	age	concrete_compressive_
1	540.0	0.0	0.0	162.0	2.5	1055.0	676.0	28	6
2	332.5	142.5	0.0	228.0	0.0	932.0	594.0	270	4
3	332.5	142.5	0.0	228.0	0.0	932.0	594.0	365	4
4	198.6	132.4	0.0	192.0	0.0	978.4	825.5	360	4

Exploratory Data Anaiysis

The dataset contains a number of features, all of which are numerical. Since all of them are components of concrete, there is a chance that two of them might be related in some way. This warrants an analysis of the data in order to gain some insights.

In [20]:

```
# Numerical exploration
pd.set_option('display.max_columns', 10)
print('Summary: \n',df.head(),'\n')
print('Shape: \n',df.shape,'\n')
print('Description: \n',df.describe(),'\n')
print('Number of unique values in each column: \n',df.nunique(axis=0),'\n')
```

```
Summary:
    cement  blast_furnace_slag  fly_ash  water  superplasticizer  \
0   540.0                 0.0      0.0  162.0               2.5
1   540.0                 0.0      0.0  162.0               2.5
2   332.5               142.5      0.0  228.0               0.0
3   332.5               142.5      0.0  228.0               0.0
4   198.6               132.4      0.0  192.0               0.0

   coarse_aggregate  fine_aggregate  age  concrete_compressive_strength
0            1040.0           676.0   28                      79.986111
1            1055.0           676.0   28                      61.887366
2             932.0           594.0  270                      40.269535
3             932.0           594.0  365                      41.052780
4             978.4           825.5  360                      44.296075

Shape:
 (1030, 9)

Description:
             cement  blast_furnace_slag      fly_ash        water  \
count  1030.000000         1030.000000  1030.000000  1030.000000
mean    281.165631           73.895485    54.187136   181.566359
std     104.507142           86.279104    63.996469    21.355567
min     102.000000            0.000000     0.000000   121.750000
25%     192.375000            0.000000     0.000000   164.900000
50%     272.900000           22.000000     0.000000   185.000000
75%     350.000000          142.950000   118.270000   192.000000
max     540.000000          359.400000   200.100000   247.000000

       superplasticizer  coarse_aggregate  fine_aggregate          age  \
count       1030.000000       1030.000000     1030.000000  1030.000000
mean           6.203112        972.918592      773.578883    45.662136
std            5.973492         77.753818       80.175427    63.169912
min            0.000000        801.000000      594.000000     1.000000
25%            0.000000        932.000000      730.950000     7.000000
50%            6.350000        968.000000      779.510000    28.000000
75%           10.160000       1029.400000      824.000000    56.000000
max           32.200000       1145.000000      992.600000   365.000000

       concrete_compressive_strength
count                    1030.000000
mean                       35.817836
std                        16.705679
min                         2.331808
25%                        23.707115
50%                        34.442774
75%                        46.136287
```

```
max                              82.599225

Number of unique values in each column:
 cement                           280
blast_furnace_slag               187
fly_ash                          163
water                            205
superplasticizer                 155
coarse_aggregate                 284
fine_aggregate                   304
age                               14
concrete_compressive_strength    938
dtype: int64
```

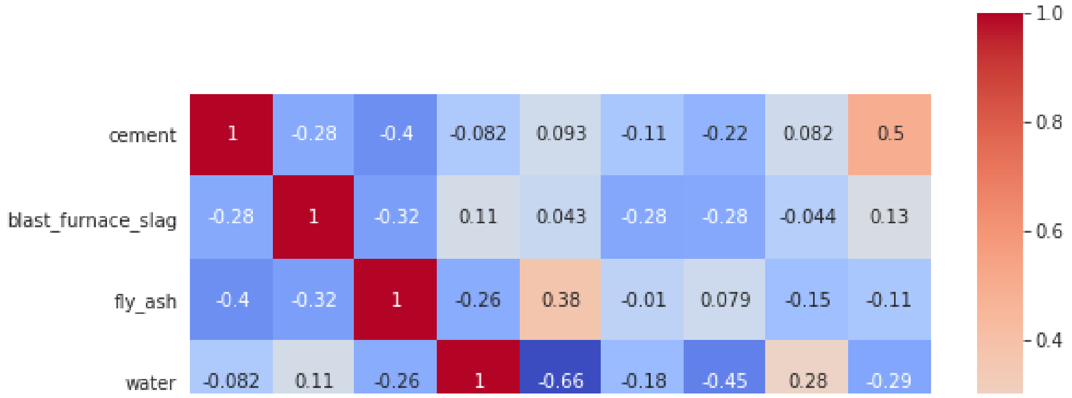
Fly Ash has median value of zero, implying it is majorly absent in concrete

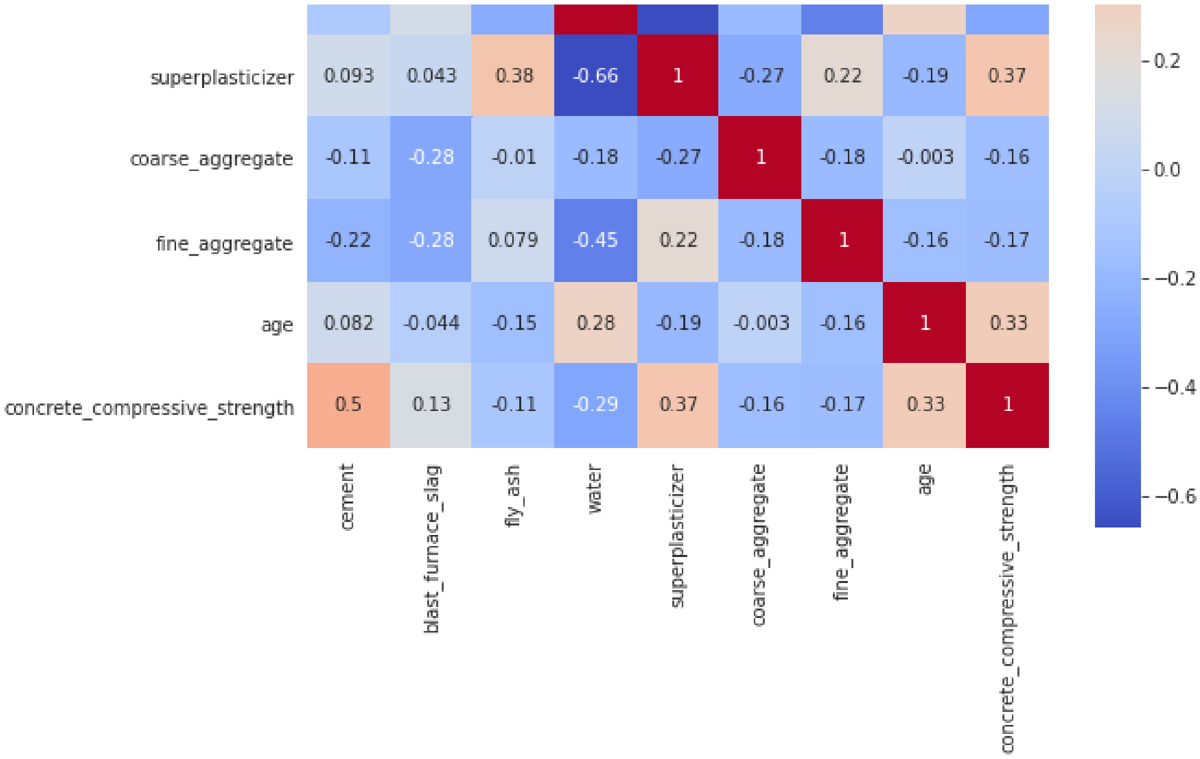
There are only 14 unique age values, but test dataset could have values not mentioned in train dataset. Thus, it is best not to categorize and encode the age column.

In [21]:

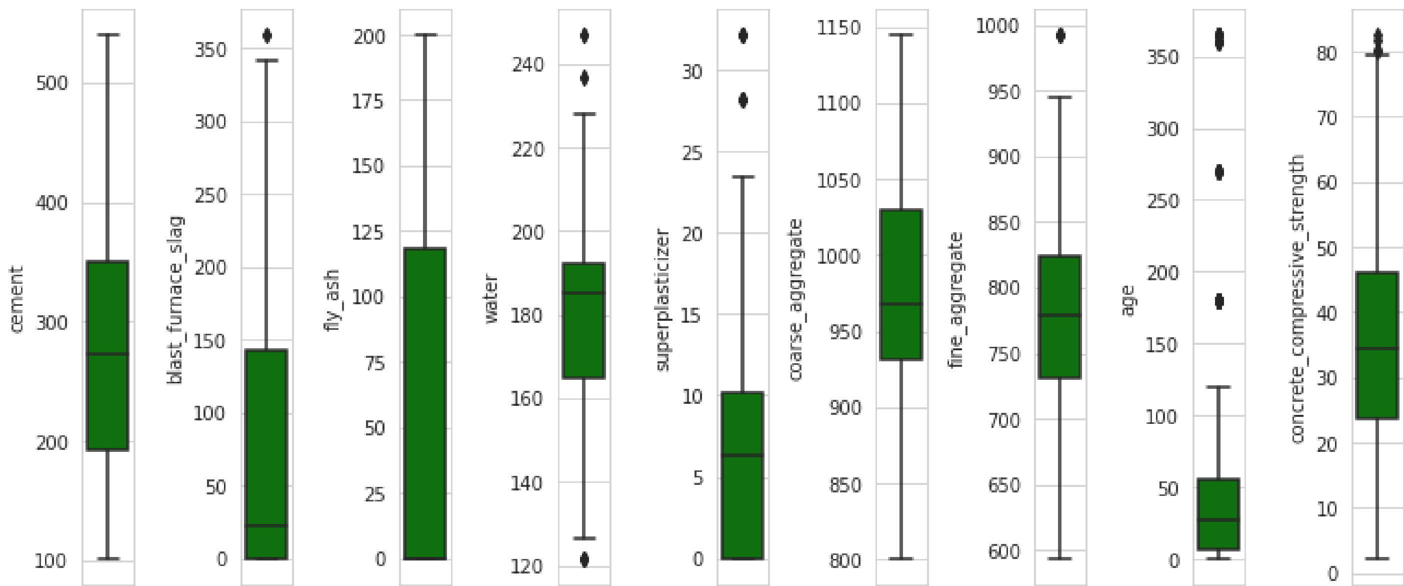
```python
# Graphical exploration

print('Correlation Heatmap: \n')
corr_matrix = df.corr()
fig, ax = plt.subplots(figsize=(9,9))
sns.heatmap(corr_matrix,cmap='coolwarm',annot=True,ax=ax,square=True)
plt.show()

l = df.columns.values
number_of_columns=len(df.columns)
number_of_rows = round(len(l)-1/number_of_columns)

print('\nBoxplots: \n')
plt.figure(figsize=(1.2*number_of_columns,5*number_of_rows))
for i in range(0,len(l)):
    plt.subplot(number_of_rows + 1,number_of_columns,i+1)
    sns.set_style('whitegrid')
    sns.boxplot(y=df[l[i]],color='green',orient='v')
    plt.tight_layout()
plt.show()

print('\nKernel Density Estimates: \n')
plt.figure(figsize=(1.5*number_of_columns,0.8*number_of_rows))
for i in range(len(l)):
    plt.subplot(2,5,i+1)
    sns.distplot(df[l[i]],kde=True)
    plt.tight_layout()
plt.show()

print('\nScatterplots: \n')
sns.pairplot(df)
plt.show()
```

```
Correlation Heatmap:
```

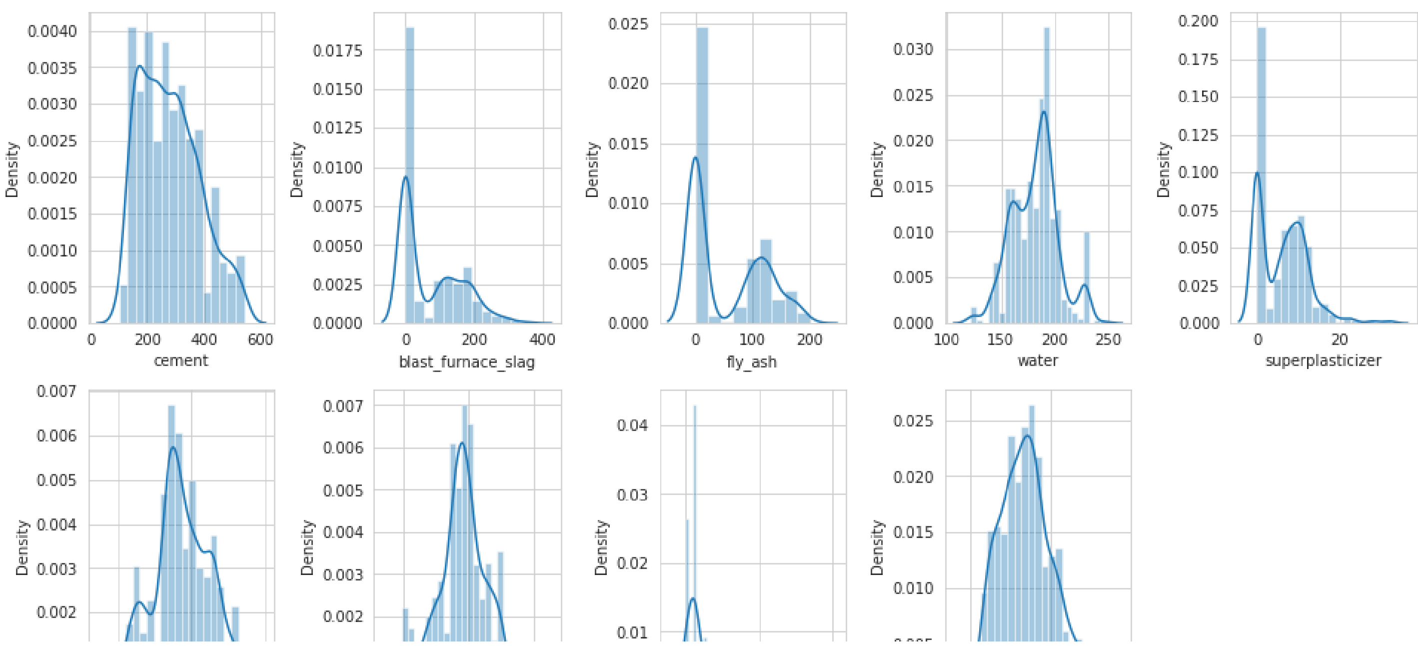


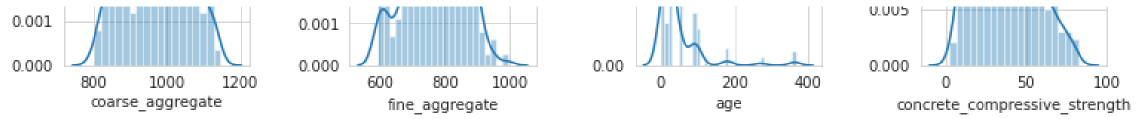


Boxplots:

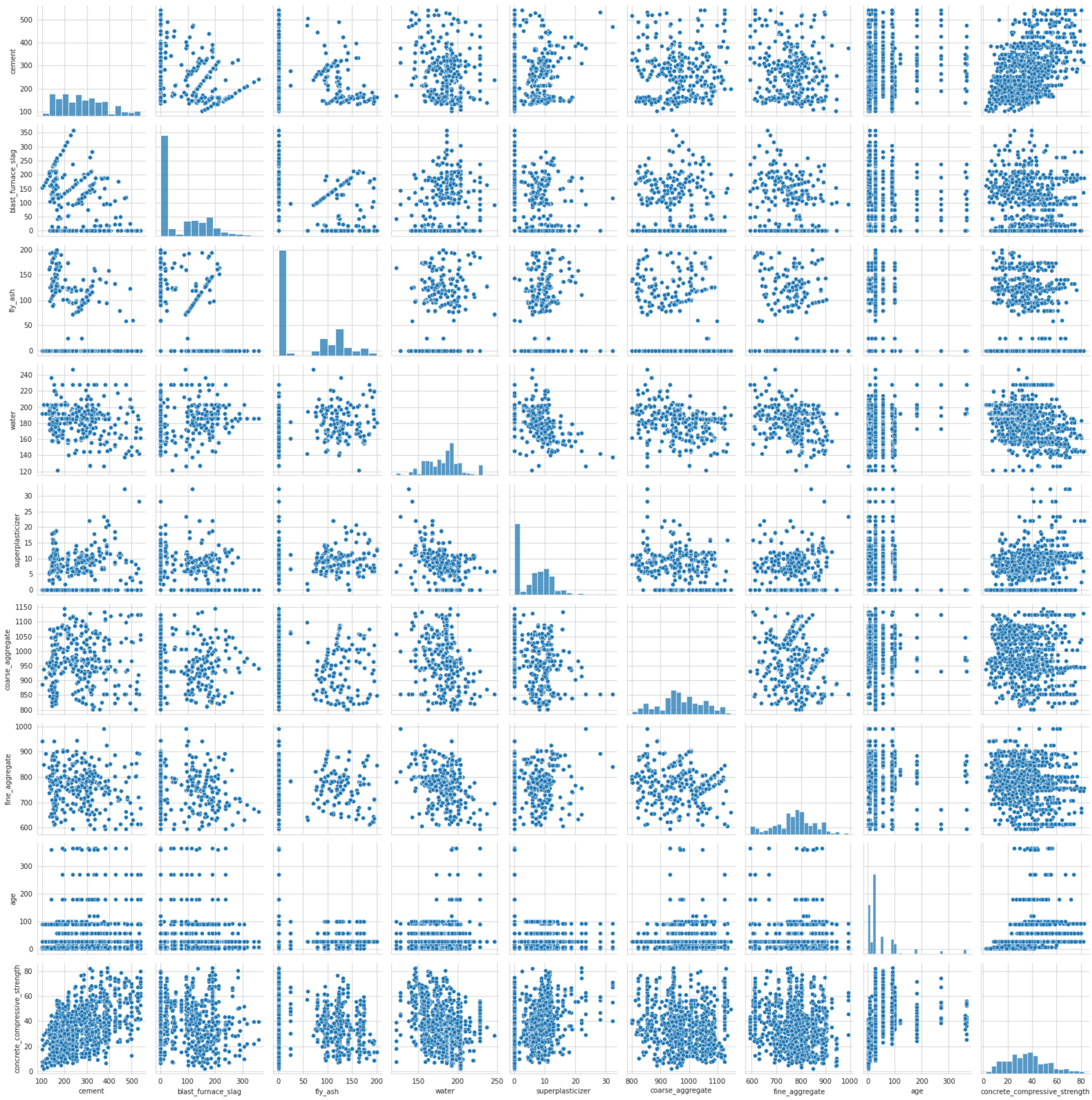


Kernel Density Estimates:






```
Scatterplots:
```



A number of insights can be gained from the visual exploration of the data.

The correlation heatmap shows the correlation between all the features. A positive correlation implies direct proportion while a negative one implies an indirect proportion. We can observe that water and superplasticizer are decently negatively correlated. This implies that the two features can be combined in some way to reduce the number of features while retaining the information. The scatter plots further elaborate the correlation map by plotting the relation between any two features.

KDE plots show the distribution of each feature. It can be seen that cement, blast furnace slag, fly ash and superplasticizer are not distributed in a Gaussian form, while the rest of them mostly are. Many machine learning models require the data to be normally distributed for best performance. This warrants using normalizing or standardizing techniques.

Boxplots are useful in understanding the general range of each feature. As observed in numerical exploration, fly ash has a median value of zero, implying it is absent in cement more than half the time. Most features have very

few outliers, except age.

Scaling and PCA

In [22]:

```
# Separate dataframe into features and labels
X = df.drop(['concrete_compressive_strength'],axis=1)
y = df['concrete_compressive_strength']
```

In [23]:

```
# Split data into train, val, test
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.3, random_state=
42, shuffle=True)
print(len(X_train),len(X_test))
```

```
721 309
```

In [24]:

```
# Scale features
scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)
print(np.mean(X_train),np.std(X_train))

# Convert standardized array to table
feat_cols = df.columns[:-1]
X_train = pd.DataFrame(X_train,columns=feat_cols)
X_test = pd.DataFrame(X_test,columns=feat_cols)
X_train.head()
```

```
2.40984609367319e-17 1.0
```

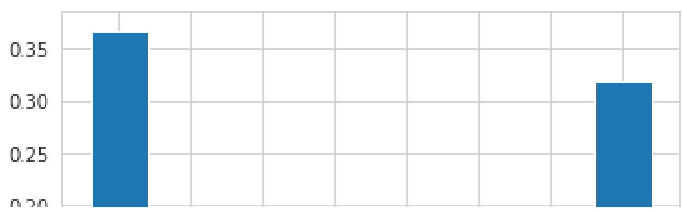
Out[24]:

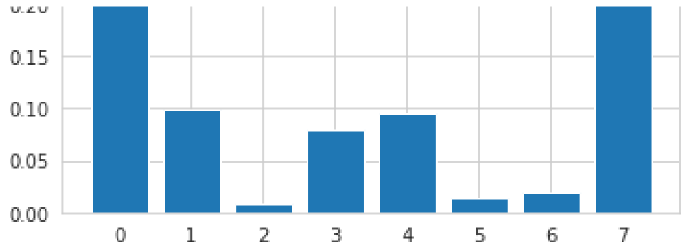
	cement	blast_furnace_slag	fly_ash	water	superplasticizer	coarse_aggregate	fine_aggregate	age
0	-0.828635	-0.855292	0.762033	-0.765446	0.224201	0.415550	1.676831	-0.292980
1	0.374843	-0.855292	-0.816902	0.103778	-1.013764	1.136985	0.141922	-0.633845
2	0.317587	1.568944	-0.816902	-1.234582	1.352934	-1.551189	1.358359	-0.698772
3	0.688826	-0.638537	1.397879	-1.314978	0.791878	-0.405305	0.366726	-0.698772
4	-1.130428	1.312260	1.507833	-0.132681	2.130800	-1.730910	-0.382619	-0.292980

We have used StandardScaler to scale the features, since their original ranges were too drastic from each other. This also brings the mean to zero and standard deviation to 1. Since we discussed that some of the features show correlation, it is important to perform feature selection to choose the most important features that retain the most information. We can use a simple Decision Tree regressor in order to extract feature importances.

In [25]:

```
# Feature Selection
model = DecisionTreeRegressor()
model.fit(X_train,y_train)
importances = model.feature_importances_
plt.bar([x for x in range(len(importances))], importances)
plt.show()
```





The bar plot shows the relative importance of each feature. Features 0, 1, 3, 4, 7 have the most importance. Together, they account for more than 95% of the total information present in the data. Thus, they are selected as the features for model training.

In [26]:

```
X_train = X_train.iloc[:,[0,1,3,4,7]]
X_test = X_test.iloc[:,[0,1,3,4,7]]
X_train.head()
```

Out[26]:

	cement	blast_furnace_slag	water	superplasticizer	age
0	-0.828635	-0.855292	-0.765446	0.224201	-0.292980
1	0.374843	-0.855292	0.103778	-1.013764	-0.633845
2	0.317587	1.568944	-1.234582	1.352934	-0.698772
3	0.688826	-0.638537	-1.314978	0.791878	-0.698772
4	-1.130428	1.312260	-0.132681	2.130800	-0.292980

Principal Component Analysis provides a further insight into the selected features by explaining the variance ratios among them. This allows choosing the principal components that affect the model, and leaving the features that don't.

In [27]:

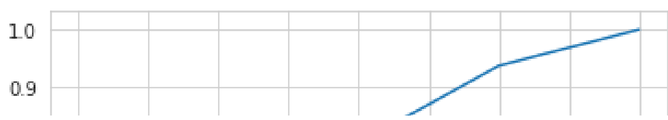
```
# Principal Component Analysis
pca = PCA()
X_pca = pca.fit_transform(X_train)
X_pca = pd.DataFrame(data = X_pca, columns = ['princ_comp'+str(i) for i in range(X_pca.s
hape[1])])
display(X_pca.head())
print('Explained variation per principal component: {}'.format(pca.explained_variance_rat
io_),'\n')
plt.plot(np.cumsum(pca.explained_variance_ratio_))
```

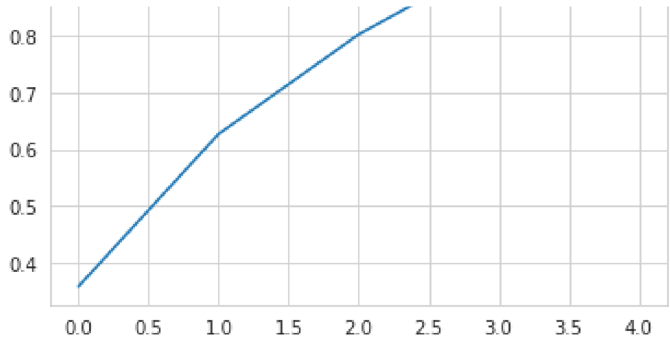
	princ_comp0	princ_comp1	princ_comp2	princ_comp3	princ_comp4
0	0.695233	-0.097289	-0.458468	1.189559	-0.148707
1	-0.364426	0.723823	-1.224048	0.002959	-0.396550
2	1.829072	-1.198107	0.674546	-1.060944	-0.209225
3	1.788710	0.582303	-0.363462	-0.020571	-0.235885
4	1.238509	-1.932557	0.995136	0.051666	1.175585

```
Explained variation per principal component: [0.358847   0.26772191 0.17488003 0.13537616
0.0631749 ]
```

Out[27]:

```
[<matplotlib.lines.Line2D at 0x7fcc1dfde510>]
```





Since the explained variation per principal component is not drastically different, all the principal components are kept for further analysis. Although, an argument can be made to disregard the last principal component due to its low variation.

In [28]:

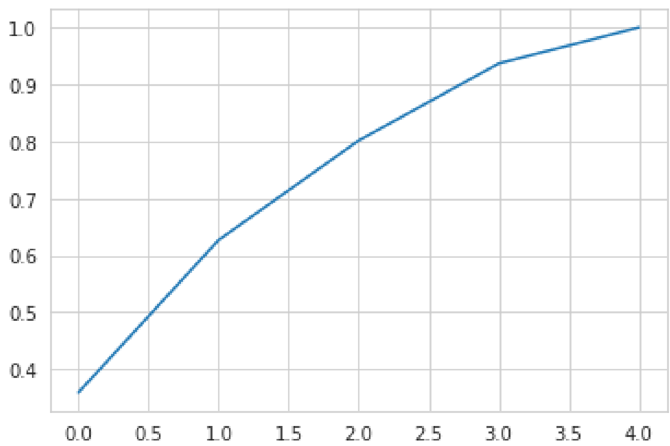
```
# Principal Component Analysis, selecting components
pca = PCA(n_components=5)
X_train = pca.fit_transform(X_train)
X_test = pca.transform(X_test)
X_train = pd.DataFrame(data = X_train, columns = ['princ_comp'+str(i) for i in range(X_train.shape[1])])
X_test = pd.DataFrame(data = X_test, columns = ['princ_comp'+str(i) for i in range(X_test.shape[1])])

display(X_train.head())
print('Explained variation per principal component: {}'.format(pca.explained_variance_ratio_),'\n')
plt.plot(np.cumsum(pca.explained_variance_ratio_))
```

	princ_comp0	princ_comp1	princ_comp2	princ_comp3	princ_comp4
0	0.695233	-0.097289	-0.458468	1.189559	-0.148707
1	-0.364426	0.723823	-1.224048	0.002959	-0.396550
2	1.829072	-1.198107	0.674546	-1.060944	-0.209225
3	1.788710	0.582303	-0.363462	-0.020571	-0.235885
4	1.238509	-1.932557	0.995136	0.051666	1.175585

```
Explained variation per principal component: [0.358847   0.26772191 0.17488003 0.13537616
 0.0631749 ]
```

Out[28]:

```
[<matplotlib.lines.Line2D at 0x7fcc1de86590>]
```



Build Model

Now, we can use different regression models and test their performance. Different types of scoring are available

for regression analyses. We use three: mean absolute error, root mean square error and r2 score. These are sufficient to estimate the performance of the model.

In [29]:

```
# Linear Regression
regressor = LinearRegression()
regressor.fit(X_train,y_train)
y_pred = regressor.predict(X_test)
print(f'Mean Absolute Error: {mean_absolute_error(y_test, y_pred)}\n')
print(f'Root Mean Square Error: {np.sqrt(mean_squared_error(y_test, y_pred))}\n')
print(f'R2 Score: {r2_score(y_test, y_pred)}\n')
print(cross_val_score(regressor, X_train, y_train, cv=5, scoring = 'r2').mean(),'\n')
print(cross_val_score(regressor, X_test, y_test, cv=5, scoring = 'r2').mean())
```

```
Mean Absolute Error: 8.907708925191603

Root Mean Square Error: 11.026404026406352

R2 Score: 0.5506599203032488

0.5776539948029964

0.5476240609244898
```

In [30]:

```
# Decision Tree Regression
regressor = DecisionTreeRegressor(max_depth=8,random_state=42)
regressor.fit(X_train,y_train)
y_pred = regressor.predict(X_test)
print(f'Mean Absolute Error: {mean_absolute_error(y_test, y_pred)}\n')
print(f'Root Mean Square Error: {np.sqrt(mean_squared_error(y_test, y_pred))}\n')
print(f'R2 Score: {r2_score(y_test, y_pred)}\n')
print(cross_val_score(regressor, X_train, y_train, cv=5, scoring = 'r2').mean(),'\n')
print(cross_val_score(regressor, X_test, y_test, cv=5, scoring = 'r2').mean())
```

```
Mean Absolute Error: 6.692775509639123

Root Mean Square Error: 9.143187640634169

R2 Score: 0.6910397414786145

0.6877090313381521

0.5339199324716439
```

In [31]:

```
# Random Forest Regression
regressor = RandomForestRegressor(n_estimators=100, max_depth=12, random_state=42)
regressor.fit(X_train,y_train)
y_pred = regressor.predict(X_test)
print(f'Mean Absolute Error: {mean_absolute_error(y_test, y_pred)}\n')
print(f'Root Mean Square Error: {np.sqrt(mean_squared_error(y_test, y_pred))}\n')
print(f'R2 Score: {r2_score(y_test, y_pred)}\n')
print(cross_val_score(regressor, X_train, y_train, cv=5, scoring = 'r2').mean(),'\n')
print(cross_val_score(regressor, X_test, y_test, cv=5, scoring = 'r2').mean())
```

```
Mean Absolute Error: 5.480738181113768

Root Mean Square Error: 7.184776940795149

R2 Score: 0.8092195215475113

0.8288832399885354

0.7153792731731963
```

Conclusion

We can see from these three models that Linear Regression is inefficient with an r2 score of only around 0.55, Decision Tree Regression is better with an r2 score reaching 0.75, and Random Forest Regression performs the best with an r2 score of 0.82.

The errors estimate the difference between the predicted concrete strength and the given strength. Lower the error, better the model. This is observable from the performance of the three models: Random Forest Regressor gives the least error.

There are a number of ways to improve the performance of these models. As mentioned in PCA, the last component can be disregarded and the models can be tested on a smaller dataset with only four principal components. Alternatively, the features removed during feature importance can be included to check if we are correct in removing them for further analysis. The order of processing: - Scaling, Feature Selection, PCA - is also a rule of thumb. Performing feature selection before scaling can lead to very different results. Finally, ensemble methods, stacking, boosting, etc. are various methods that can improve the model performance.