regression-final-assignment

December 30, 2023

```python
[27]: import pandas as pd
      import re
      import matplotlib.pyplot as plt
      import seaborn as sns
      import plotly.express as px
      import numpy as np

      from sklearn.linear_model import LinearRegression
      from sklearn.ensemble import RandomForestRegressor
      from xgboost import XGBRegressor as xgb

      from sklearn.preprocessing import StandardScaler
      from sklearn.model_selection import train_test_split

      from sklearn.model_selection import RandomizedSearchCV

      from sklearn.metrics import mean_absolute_error, mean_squared_error, r2_score
```

0.0.1 Dataset Overview

```python
[2]: data = pd.read_csv("concrete.csv")
```

```python
[3]: data.head()
```

```
[3]:    Cement (component 1)(kg in a m^3 mixture)  \
    0                                      540.0
    1                                      540.0
    2                                      332.5
    3                                      332.5
    4                                      198.6

       Blast Furnace Slag (component 2)(kg in a m^3 mixture)  \
    0                                                0.0
    1                                                0.0
    2                                              142.5
    3                                              142.5
    4                                              132.4
```

```
   Fly Ash (component 3)(kg in a m^3 mixture)  \
0                                         0.0
1                                         0.0
2                                         0.0
3                                         0.0
4                                         0.0

   Water  (component 4)(kg in a m^3 mixture)  \
0                                       162.0
1                                       162.0
2                                       228.0
3                                       228.0
4                                       192.0

   Superplasticizer (component 5)(kg in a m^3 mixture)  \
0                                                 2.5
1                                                 2.5
2                                                 0.0
3                                                 0.0
4                                                 0.0

   Coarse Aggregate  (component 6)(kg in a m^3 mixture)  \
0                                              1040.0
1                                              1055.0
2                                               932.0
3                                               932.0
4                                               978.4

   Fine Aggregate (component 7)(kg in a m^3 mixture)  Age (day)  strength
0                                             676.0         28     79.99
1                                             676.0         28     61.89
2                                             594.0        270     40.27
3                                             594.0        365     41.05
4                                             825.5        360     44.30
```

[4]: `data.shape`

[4]: (1030, 9)

[5]:
```python
for col in data.columns:
    rename_col = ' '.join(re.split(r'\(', col)[0].split())
    data.rename(columns={col: rename_col}, inplace=True)
```

[6]: `data.head()`

```
[6]:    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  strength
     0            1040.0           676.0   28     79.99
     1            1055.0           676.0   28     61.89
     2             932.0           594.0  270     40.27
     3             932.0           594.0  365     41.05
     4             978.4           825.5  360     44.30
```

[7]: `data.describe()`

```
[7]:             Cement  Blast Furnace Slag      Fly Ash        Water  \
     count  1030.000000         1030.000000  1030.000000  1030.000000
     mean    281.167864           73.895825    54.188350   181.567282
     std     104.506364           86.279342    63.997004    21.354219
     min     102.000000            0.000000     0.000000   121.800000
     25%     192.375000            0.000000     0.000000   164.900000
     50%     272.900000           22.000000     0.000000   185.000000
     75%     350.000000          142.950000   118.300000   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           6.204660        972.918932      773.580485    45.662136
     std            5.973841         77.753954       80.175980    63.169912
     min            0.000000        801.000000      594.000000     1.000000
     25%            0.000000        932.000000      730.950000     7.000000
     50%            6.400000        968.000000      779.500000    28.000000
     75%           10.200000       1029.400000      824.000000    56.000000
     max           32.200000       1145.000000      992.600000   365.000000

              strength
     count  1030.000000
     mean     35.817961
     std      16.705742
     min       2.330000
     25%      23.710000
     50%      34.445000
     75%      46.135000
     max      82.600000
```

[8]: `data.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   Blast Furnace Slag 1030 non-null   float64
 2   Fly Ash            1030 non-null   float64
 3   Water              1030 non-null   float64
 4   Superplasticizer   1030 non-null   float64
 5   Coarse Aggregate   1030 non-null   float64
 6   Fine Aggregate     1030 non-null   float64
 7   Age                1030 non-null   int64
 8   strength           1030 non-null   float64
dtypes: float64(8), int64(1)
memory usage: 72.6 KB
```

0.0.2 Data Preprocessing:

```
[9]: data2 = data.copy()
```

```
[10]: #check missing values

      data.isnull().sum()
```

```
[10]: Cement              0
      Blast Furnace Slag  0
      Fly Ash             0
      Water               0
      Superplasticizer    0
      Coarse Aggregate    0
      Fine Aggregate      0
      Age                 0
      strength            0
      dtype: int64
```

Outliers

```
[11]: plt.figure(figsize=(15,15))

      for ax, col in enumerate(data.columns):
          plt.subplot(5, 6, int(ax+1))
          plt.title(col)
          sns.boxplot(x=data[col], hue=data['strength'])

      plt.tight_layout()
      plt.show()
```
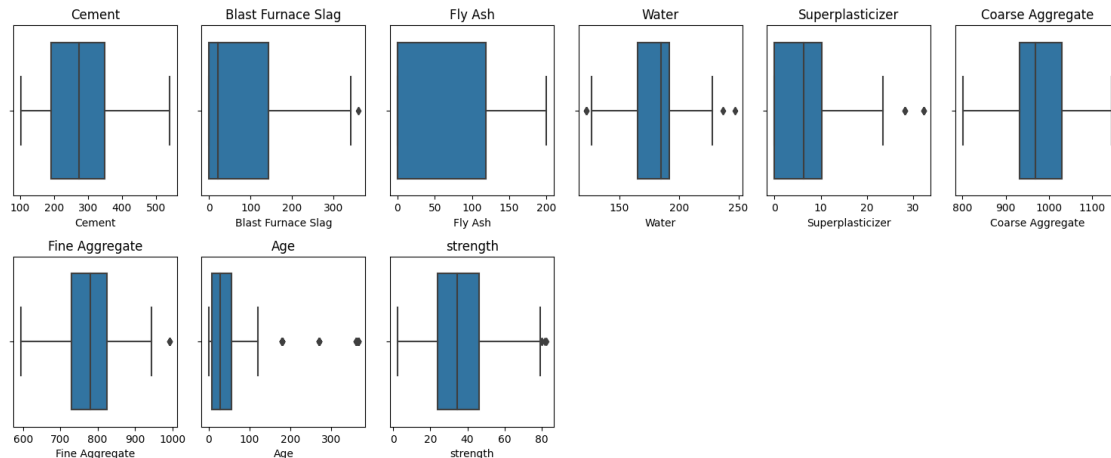
```
[12]: plt.figure(figsize=(15,15))

      for ax, col in enumerate(data.columns):
          plt.subplot(5, 6, int(ax+1))
          plt.title(col)
          sns.kdeplot(x=data[col],fill=True, hue=data['strength'])
          plt.legend()
      plt.tight_layout()
      plt.show()
```

/home/applehx7/anaconda3/lib/python3.11/site-packages/seaborn/_oldcore.py:1119:
FutureWarning: use_inf_as_na option is deprecated and will be removed in a
future version. Convert inf values to NaN before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
/tmp/ipykernel_36832/3500196248.py:6: UserWarning: Dataset has 0 variance;
skipping density estimate. Pass `warn_singular=False` to disable this warning.
  sns.kdeplot(x=data[col],fill=True, hue=data['strength'])
No artists with labels found to put in legend. Note that artists whose label
start with an underscore are ignored when legend() is called with no argument.
/home/applehx7/anaconda3/lib/python3.11/site-packages/seaborn/_oldcore.py:1119:
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```
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/tmp/ipykernel_36832/3500196248.py:6: UserWarning: Dataset has 0 variance;
skipping density estimate. Pass `warn_singular=False` to disable this warning.
```
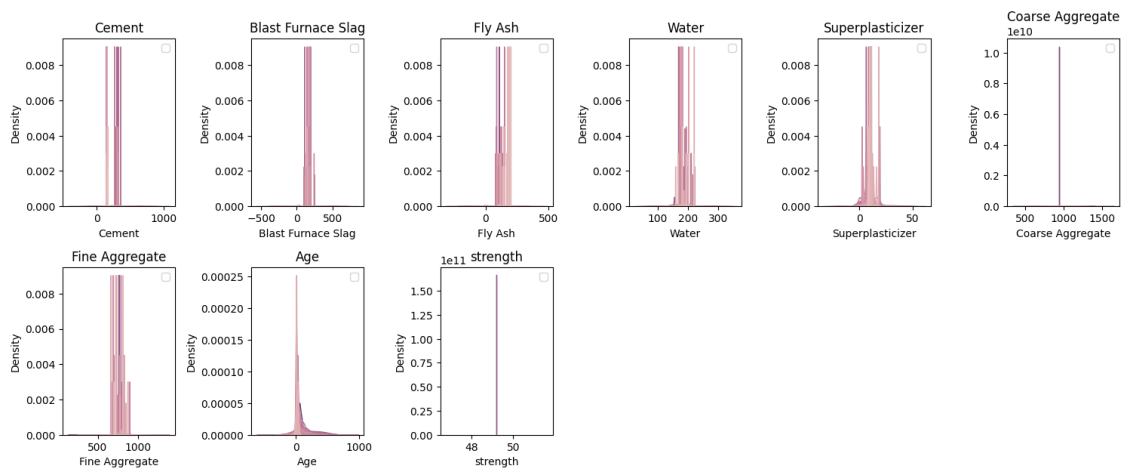
```
  sns.kdeplot(x=data[col],fill=True, hue=data['strength'])
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```
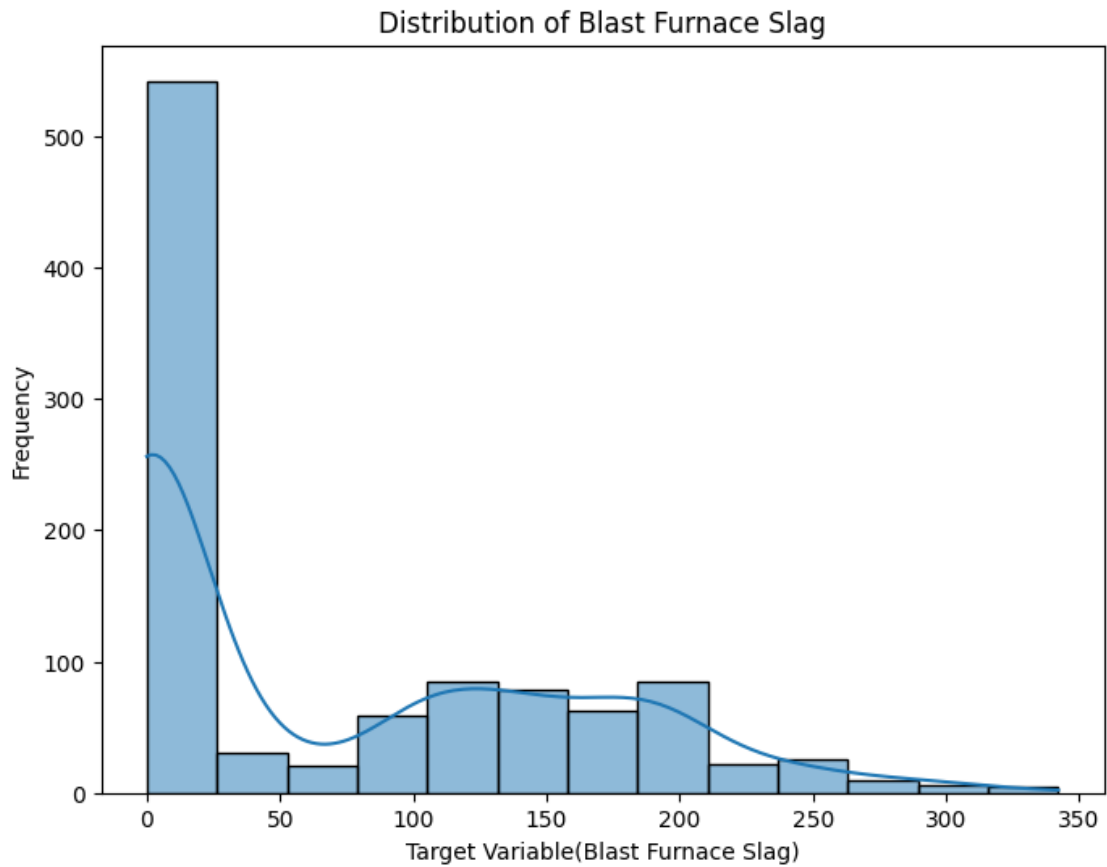

[13]:
```python
def remove_outlier(dataframe, column_name):
    Q1 = data[column_name].quantile(.25)
    Q3 = data[column_name].quantile(.75)
    IQR = Q3 - Q1
    lower_fence = Q1-(1.5*IQR)
    upper_fence = Q3 + (1.5*IQR)
    data.loc[(data[column_name] <= lower_fence), column_name] =
 ↪data[column_name].median()
    data.loc[(data[column_name] >= upper_fence), column_name] =
 ↪data[column_name].median()

def check_outliers(dataframe, column_name):
    Q1 = data[column_name].quantile(.25)
    Q3 = data[column_name].quantile(.75)
    IQR = Q3 - Q1
    lower_fence = Q1-(1.5*IQR)
    upper_fence = Q3 + (1.5*IQR)
```

7

```
    if data[(data[column_name] < lower_fence) | (data[column_name] >␣
 ↪upper_fence)].any(axis=None):
        return True
    else:
        return False
```

[14]:
```
for col in data.columns:
    print(f"{col} : {check_outliers(data, col)}")
```

```
Cement : False
Blast Furnace Slag : True
Fly Ash : False
Water : True
Superplasticizer : True
Coarse Aggregate : False
Fine Aggregate : True
Age : True
strength : True
```

[15]:
```
for col in data.columns:
    while check_outliers(data, col):
        remove_outlier(data, col)
```

0.0.3   EDA and Exploring the distribution of the target variable and features.

[16]:
```
for col in data.columns:
    plt.figure(figsize=(8, 6))
    sns.histplot(data[col], kde=True)
    plt.title(f'Distribution of {col}')
    plt.xlabel(f'Target Variable({col})')
    plt.ylabel('Frequency')
    plt.show()
```

/home/applehx7/anaconda3/lib/python3.11/site-packages/seaborn/_oldcore.py:1119:
FutureWarning: use_inf_as_na option is deprecated and will be removed in a
future version. Convert inf values to NaN before operating instead.
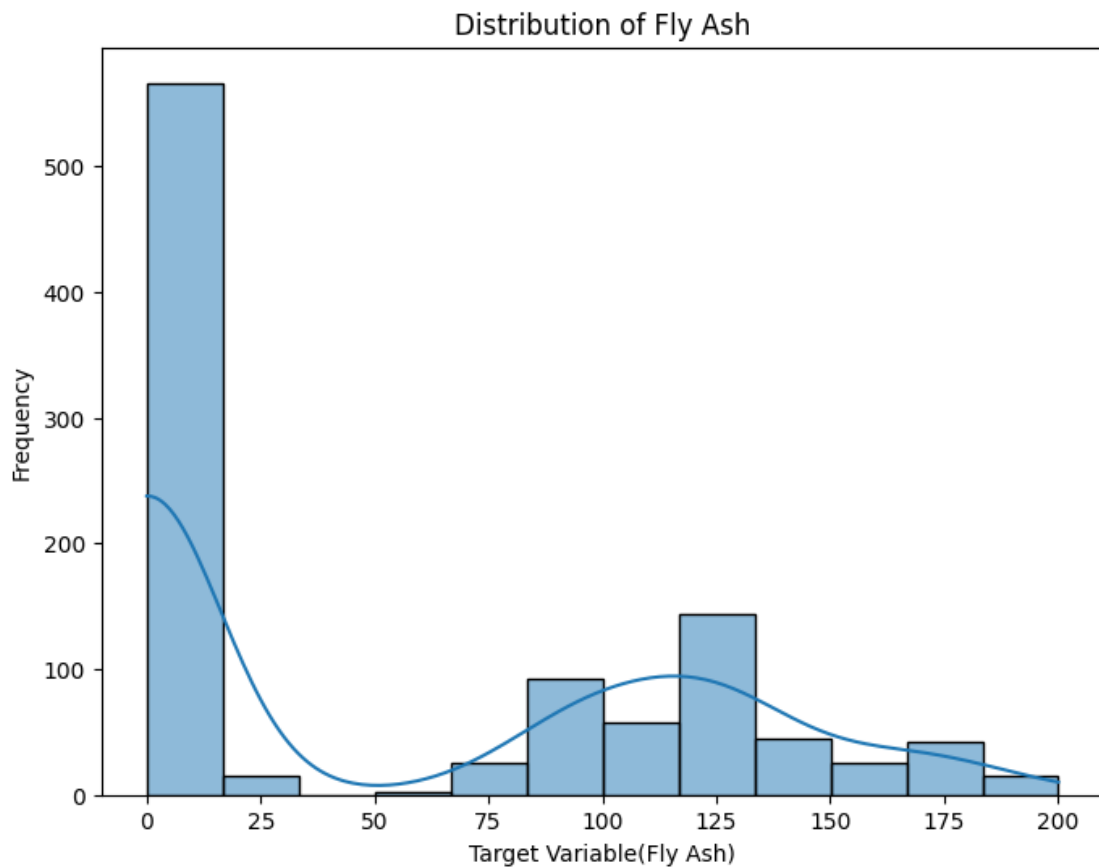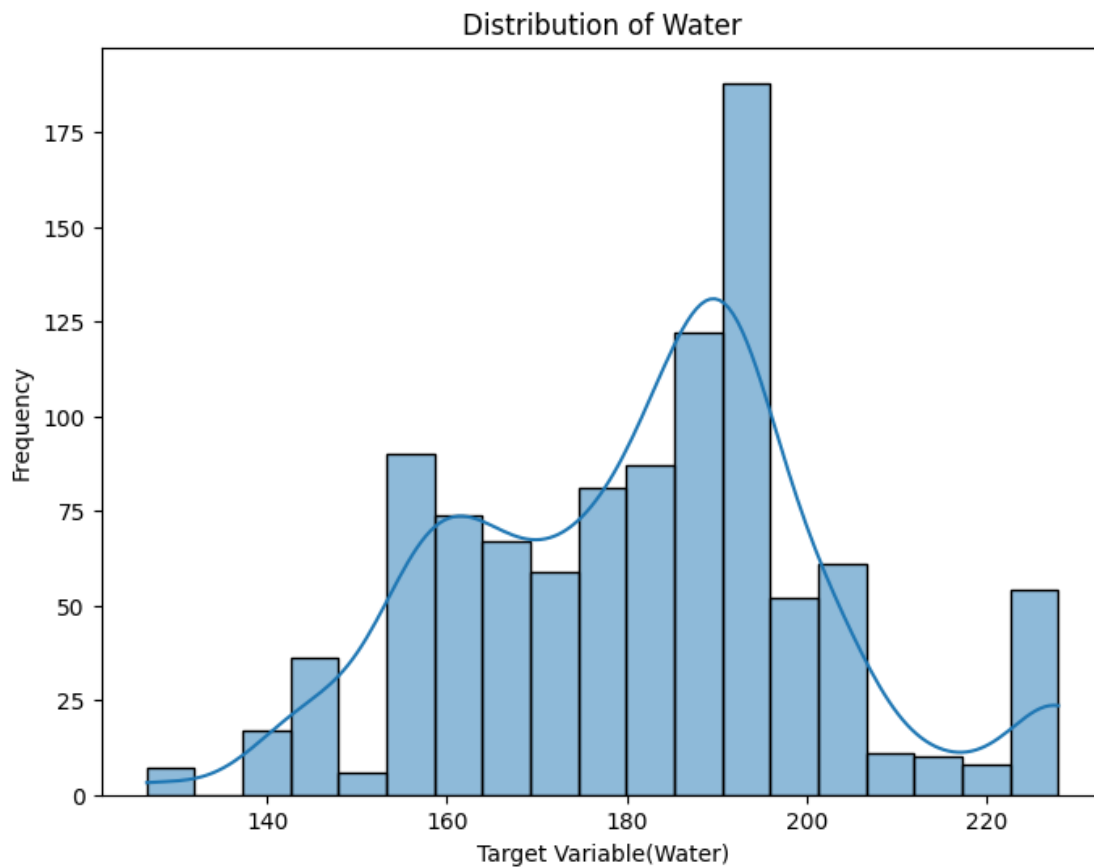 with pd.option_context('mode.use_inf_as_na', True):

Distribution of Cement
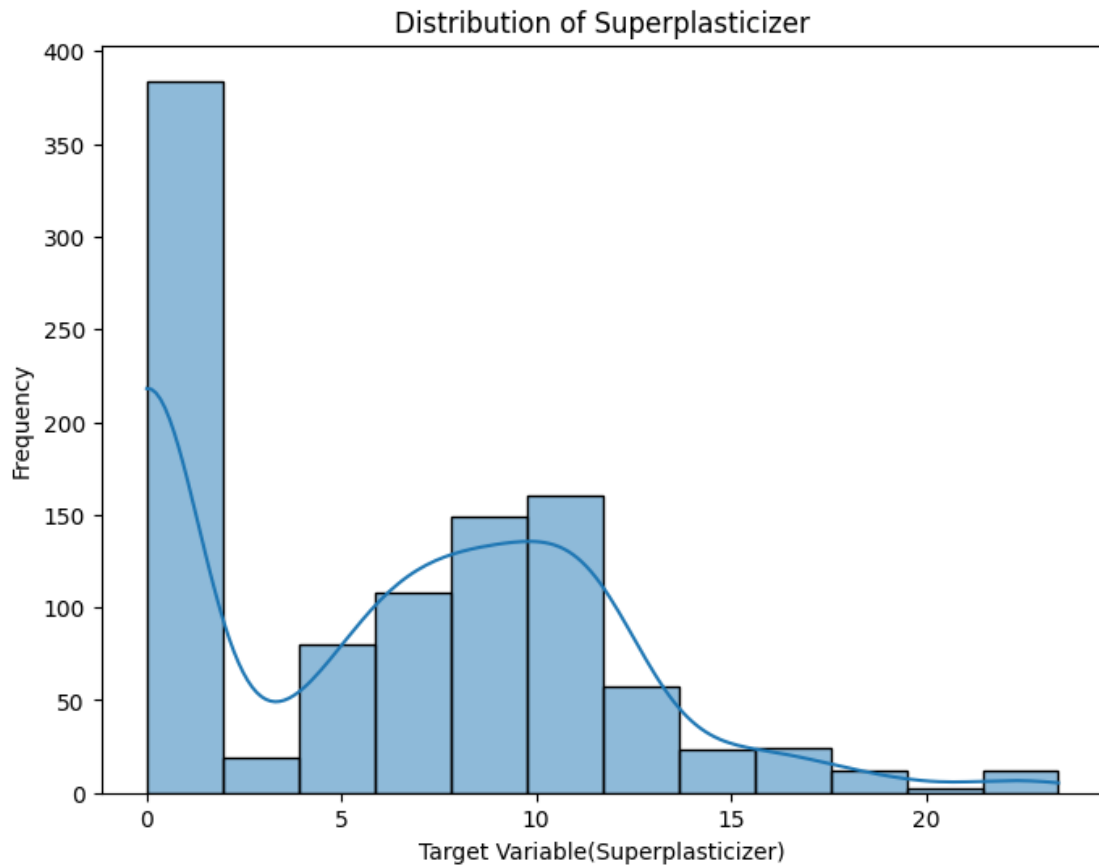
/home/applehx7/anaconda3/lib/python3.11/site-packages/seaborn/_oldcore.py:1119:
FutureWarning: use_inf_as_na option is deprecated and will be removed in a
future version. Convert inf values to NaN before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
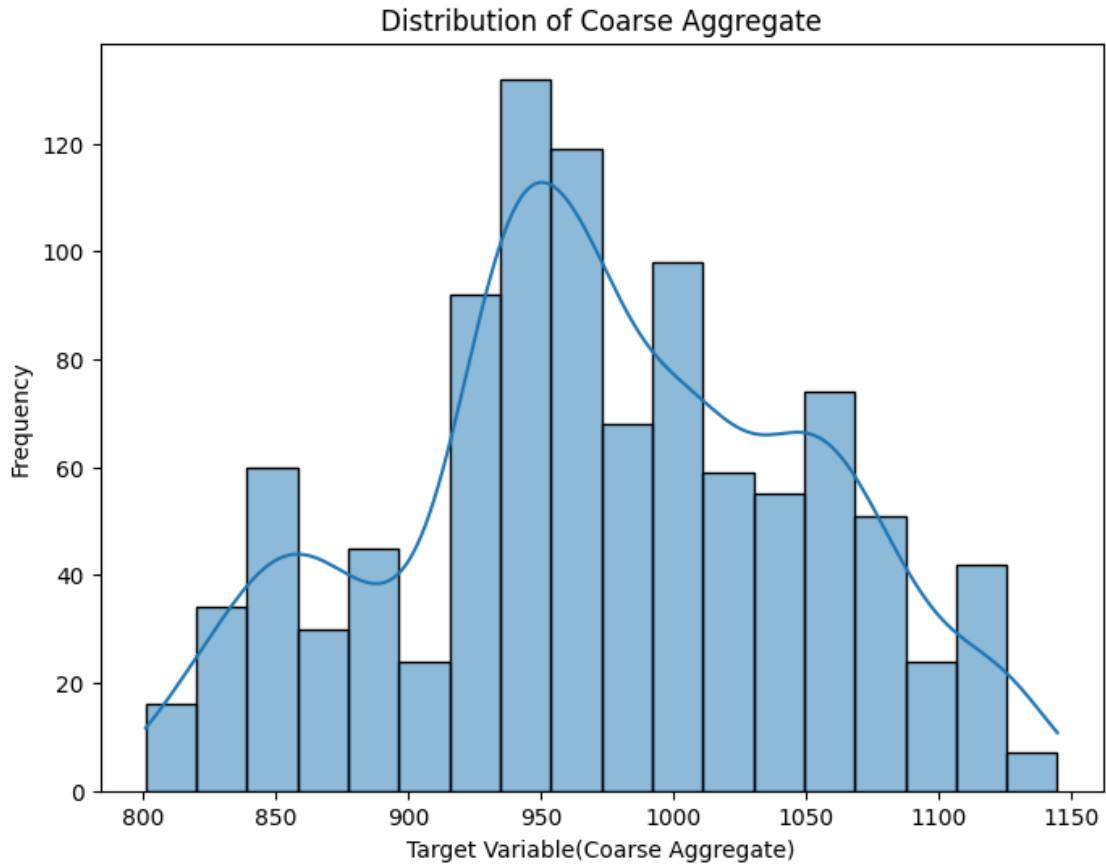
Distribution of Blast Furnace Slag

```
/home/applehx7/anaconda3/lib/python3.11/site-packages/seaborn/_oldcore.py:1119:
FutureWarning: use_inf_as_na option is deprecated and will be removed in a
future version. Convert inf values to NaN before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
```

Distribution of Fly Ash


```
/home/applehx7/anaconda3/lib/python3.11/site-packages/seaborn/_oldcore.py:1119:
FutureWarning: use_inf_as_na option is deprecated and will be removed in a
future version. Convert inf values to NaN before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
```
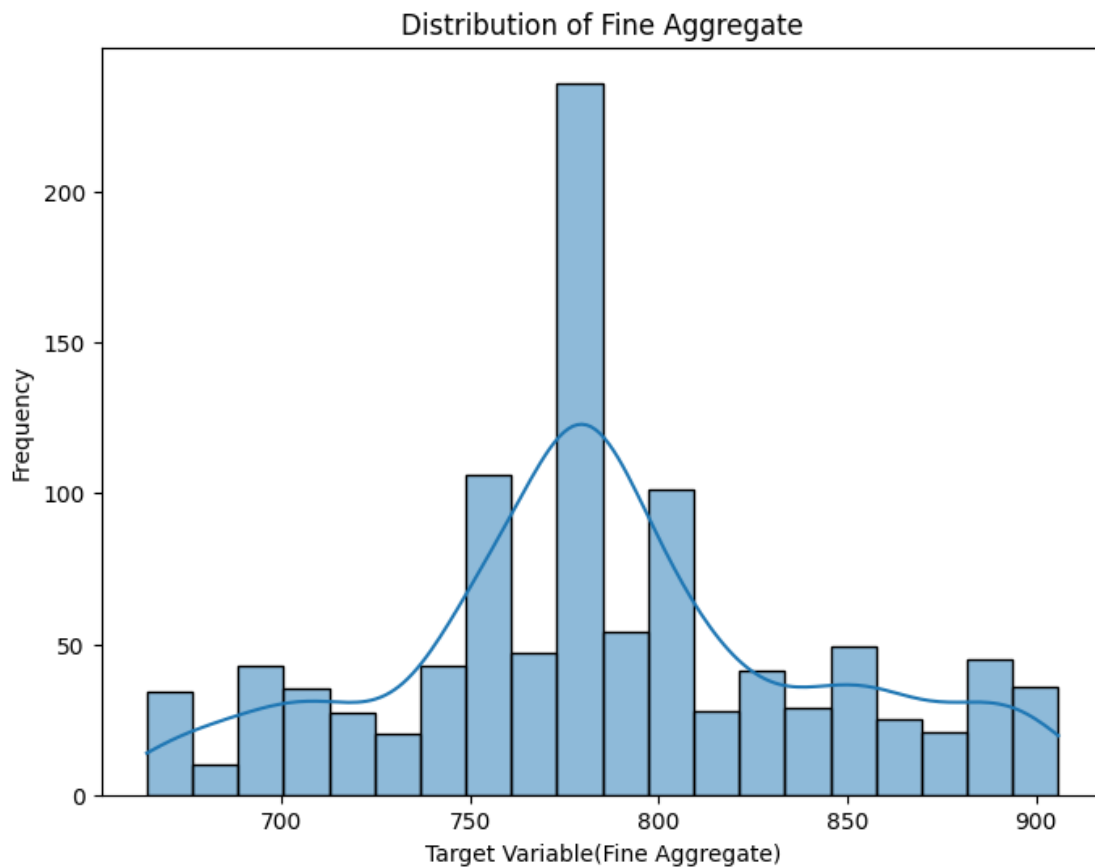
Distribution of Water

```
/home/applehx7/anaconda3/lib/python3.11/site-packages/seaborn/_oldcore.py:1119:
FutureWarning: use_inf_as_na option is deprecated and will be removed in a
future version. Convert inf values to NaN before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
```

Distribution of Superplasticizer

```
/home/applehx7/anaconda3/lib/python3.11/site-packages/seaborn/_oldcore.py:1119:
FutureWarning: use_inf_as_na option is deprecated and will be removed in a
future version. Convert inf values to NaN before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
```
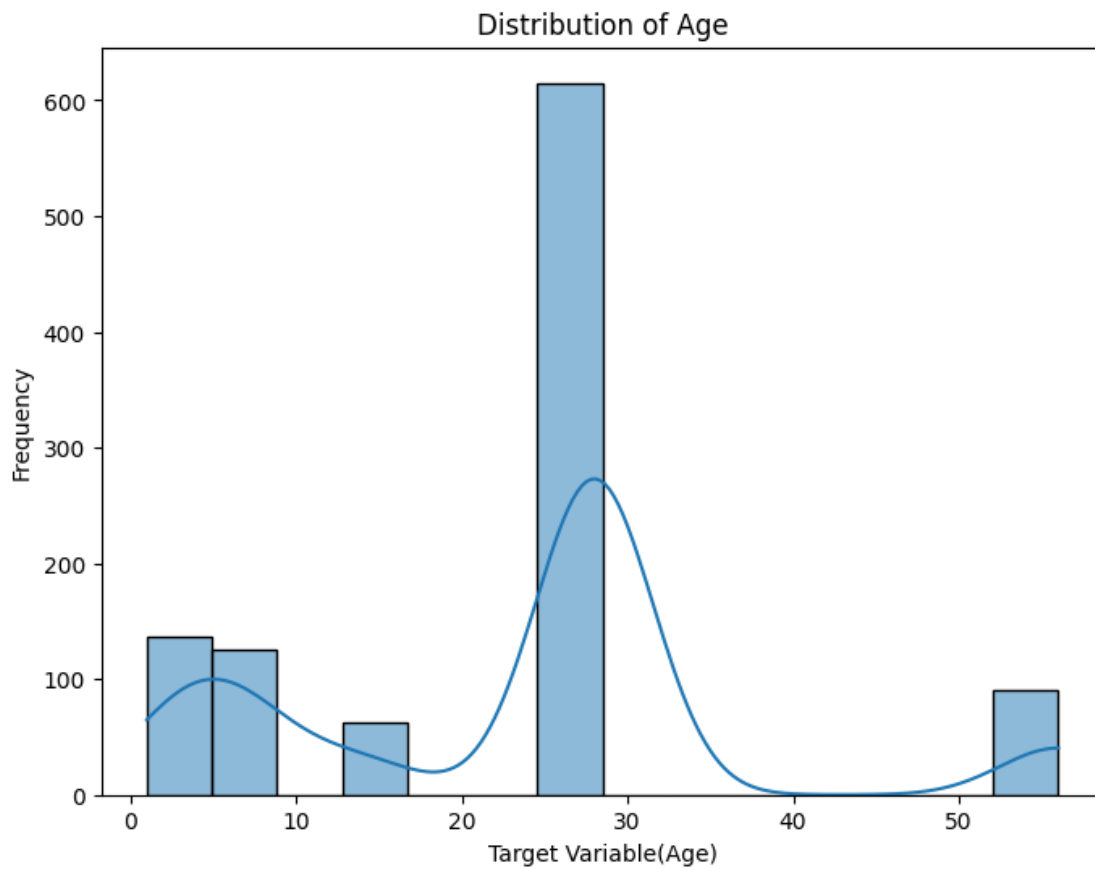
Distribution of Coarse Aggregate

/home/applehx7/anaconda3/lib/python3.11/site-packages/seaborn/_oldcore.py:1119:
FutureWarning: use_inf_as_na option is deprecated and will be removed in a
future version. Convert inf values to NaN before operating instead.
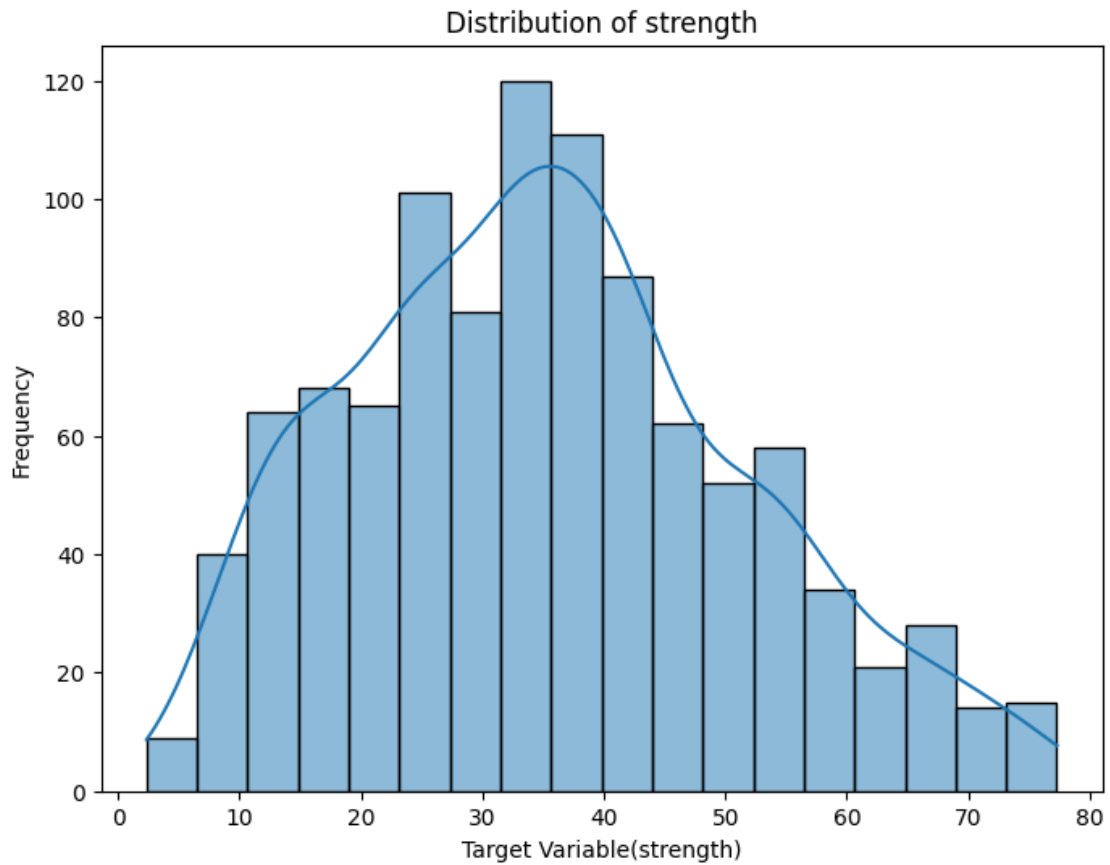 with pd.option_context('mode.use_inf_as_na', True):

Distribution of Fine Aggregate

/home/applehx7/anaconda3/lib/python3.11/site-packages/seaborn/_oldcore.py:1119:
FutureWarning: use_inf_as_na option is deprecated and will be removed in a
future version. Convert inf values to NaN before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
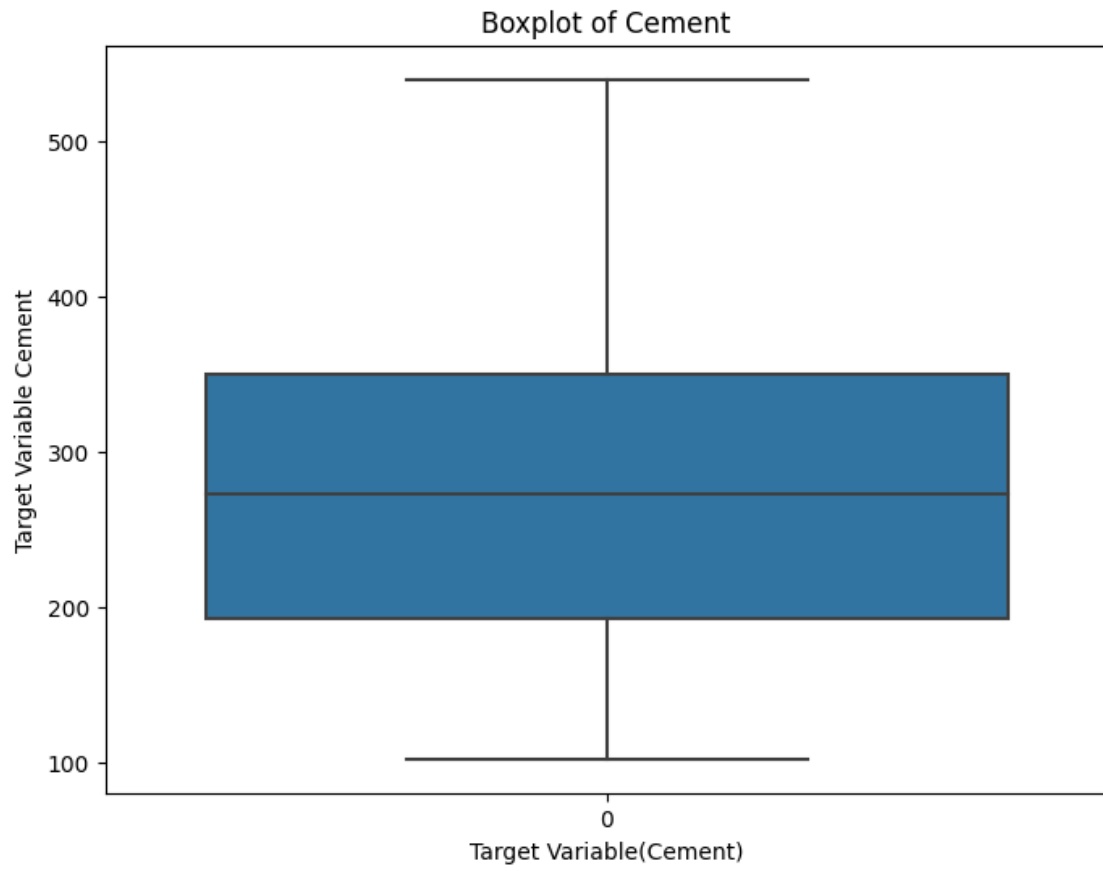
Distribution of Age

```
/home/applehx7/anaconda3/lib/python3.11/site-packages/seaborn/_oldcore.py:1119:
FutureWarning: use_inf_as_na option is deprecated and will be removed in a
future version. Convert inf values to NaN before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
```

Distribution of strength

```
for col in data.columns:
    plt.figure(figsize=(8, 6))
    sns.boxplot(data[col])
    plt.title(f'Boxplot of {col}')
    plt.ylabel(f'Target Variable {col}')
    plt.xlabel(f'Target Variable({col})')
    plt.show()
```

Boxplot of Cement

Boxplot of Blast Furnace Slag

Boxplot of Fly Ash

Boxplot of Water

Boxplot of Superplasticizer

Boxplot of Coarse Aggregate

Boxplot of Fine Aggregate

Boxplot of Age

Boxplot of strength
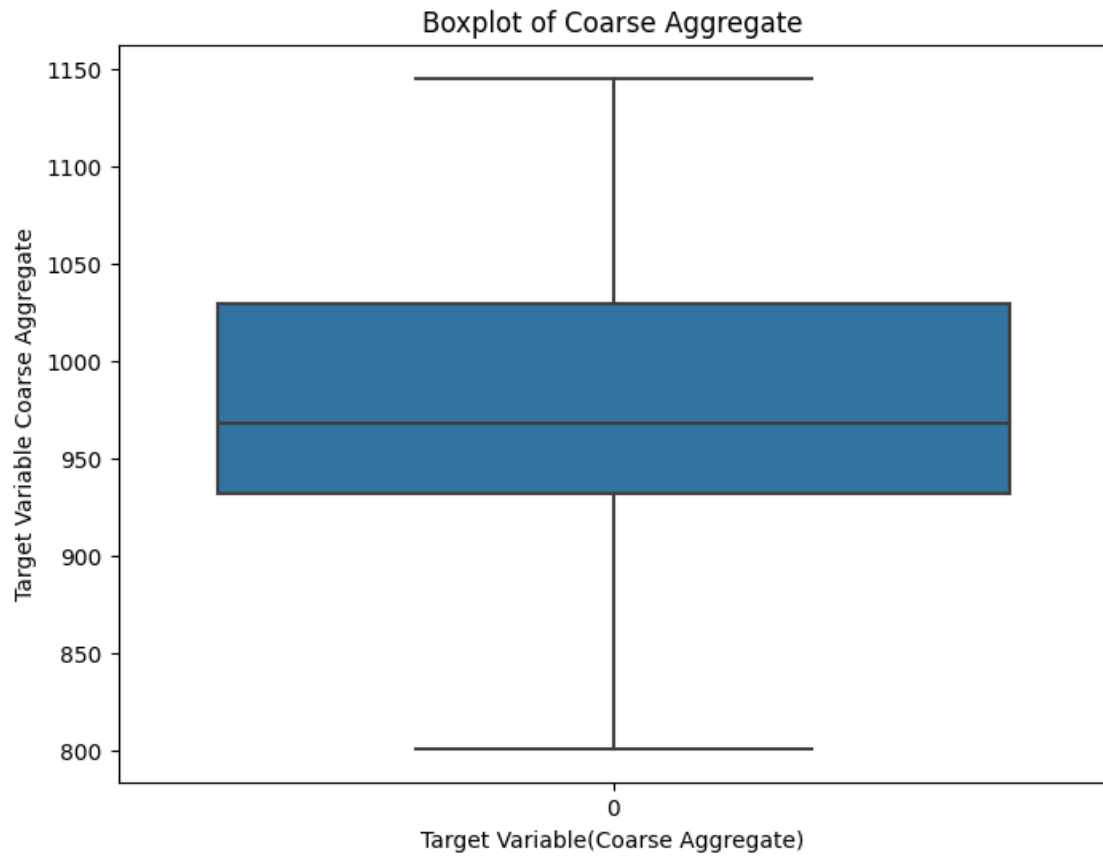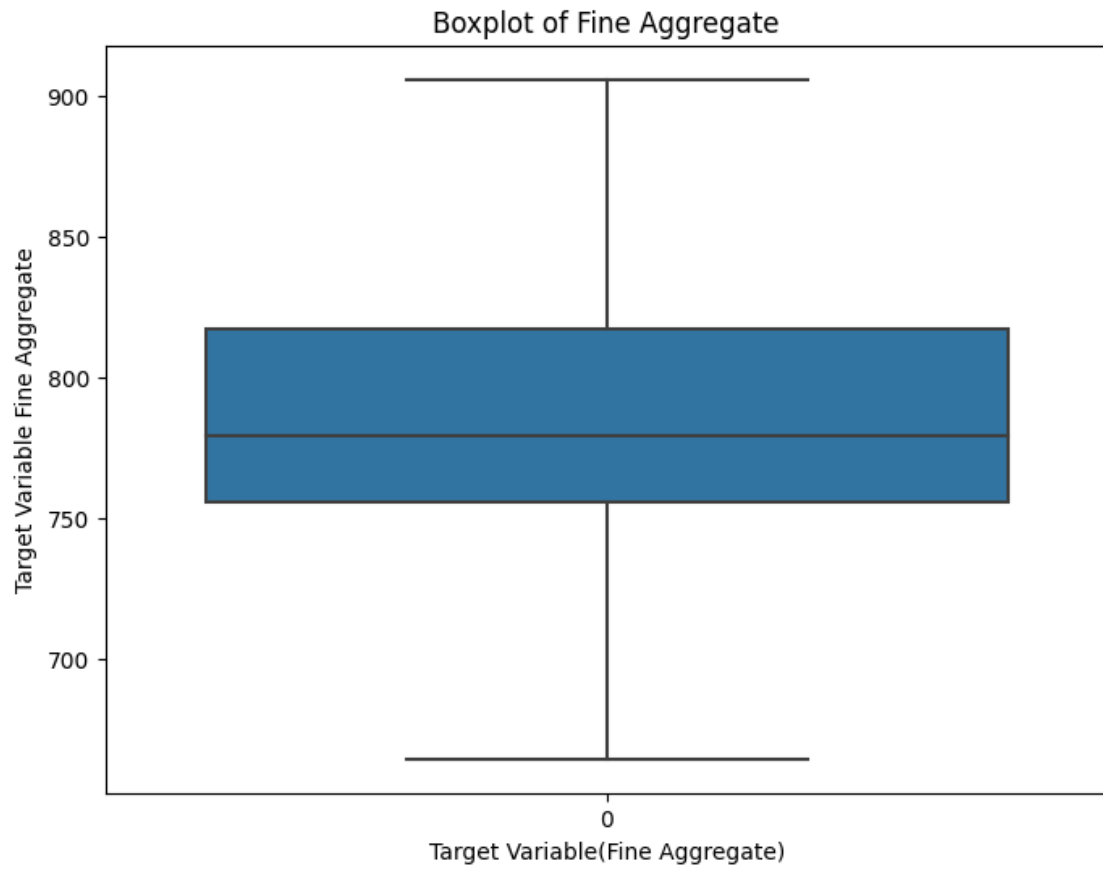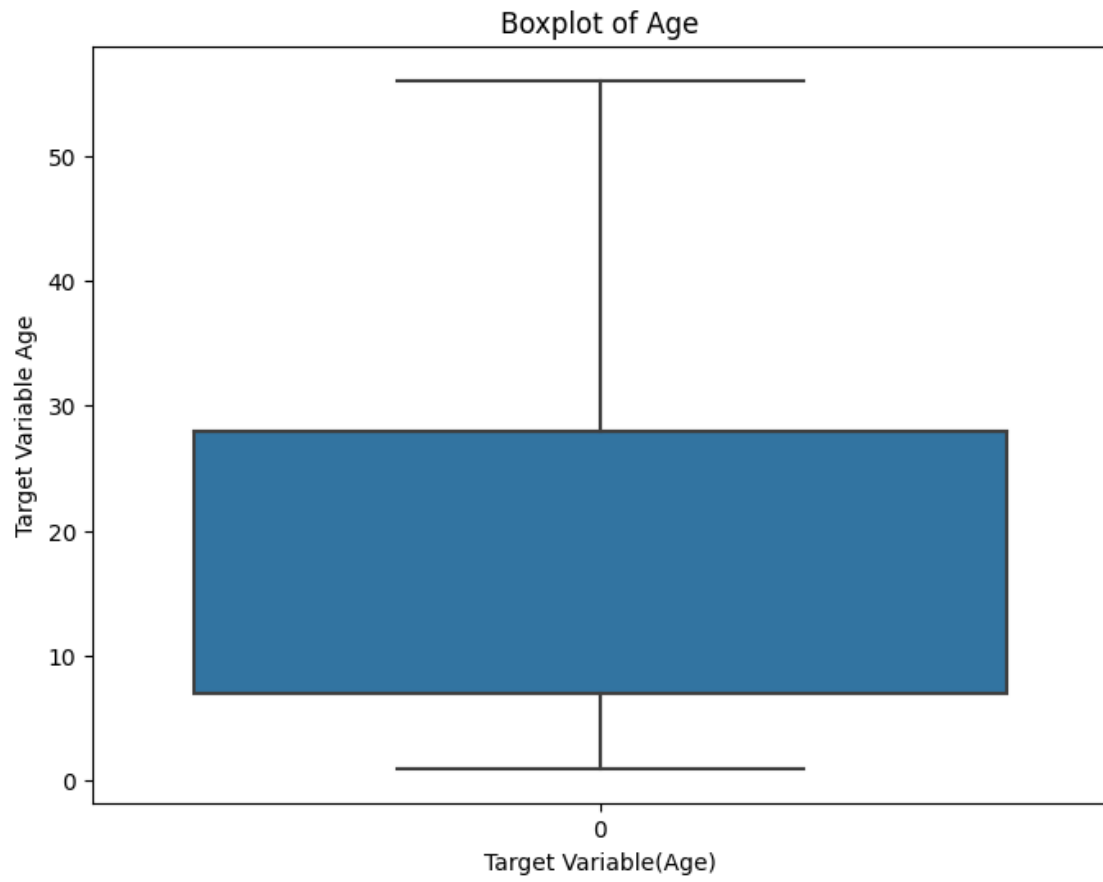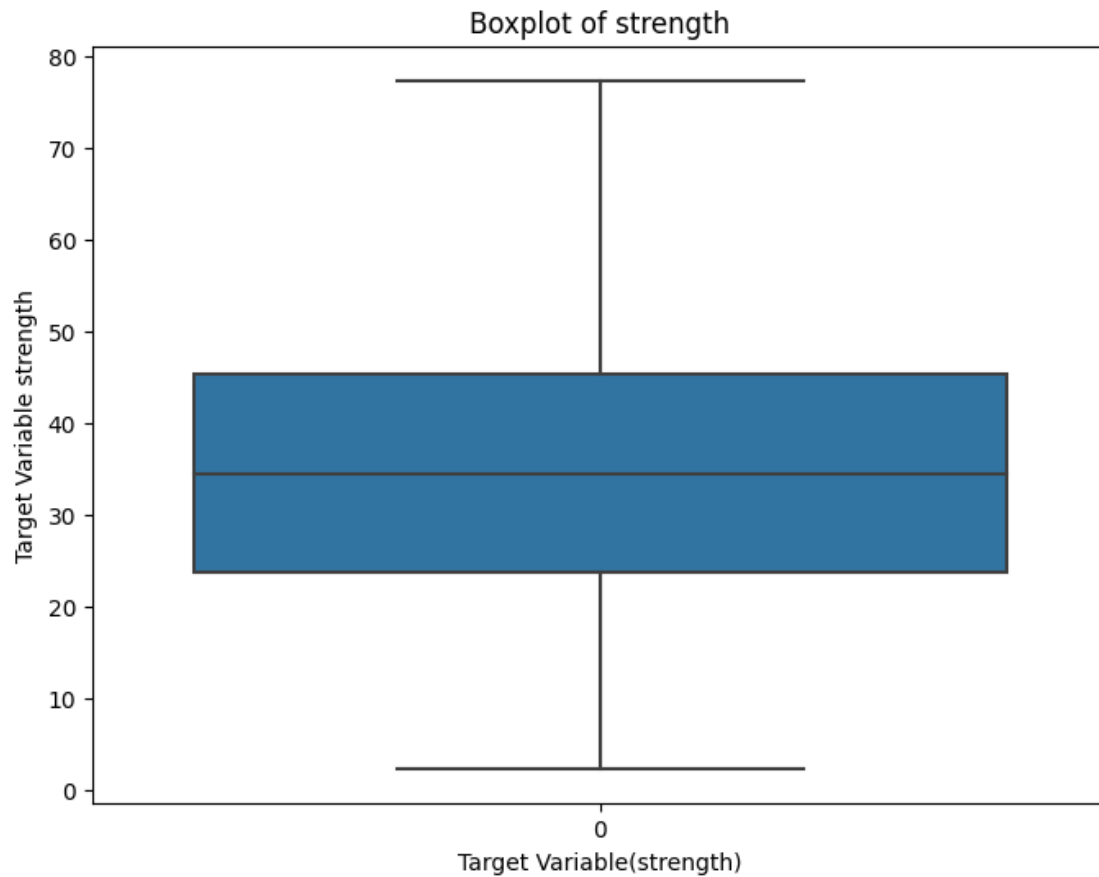
```
[18]: for col in data.columns:
          plt.figure(figsize=(8, 6))
          sns.scatterplot(x=data[col], y=data['strength'])
          plt.title(f'{col} vs. Strength')
          plt.xlabel(col)
          plt.ylabel('Strength')
          plt.show()
```

Cement vs. Strength

Blast Furnace Slag vs. Strength

Fly Ash vs. Strength

Water vs. Strength

Superplasticizer vs. Strength

Coarse Aggregate vs. Strength

Fine Aggregate vs. Strength

Age vs. Strength

strength vs. Strength
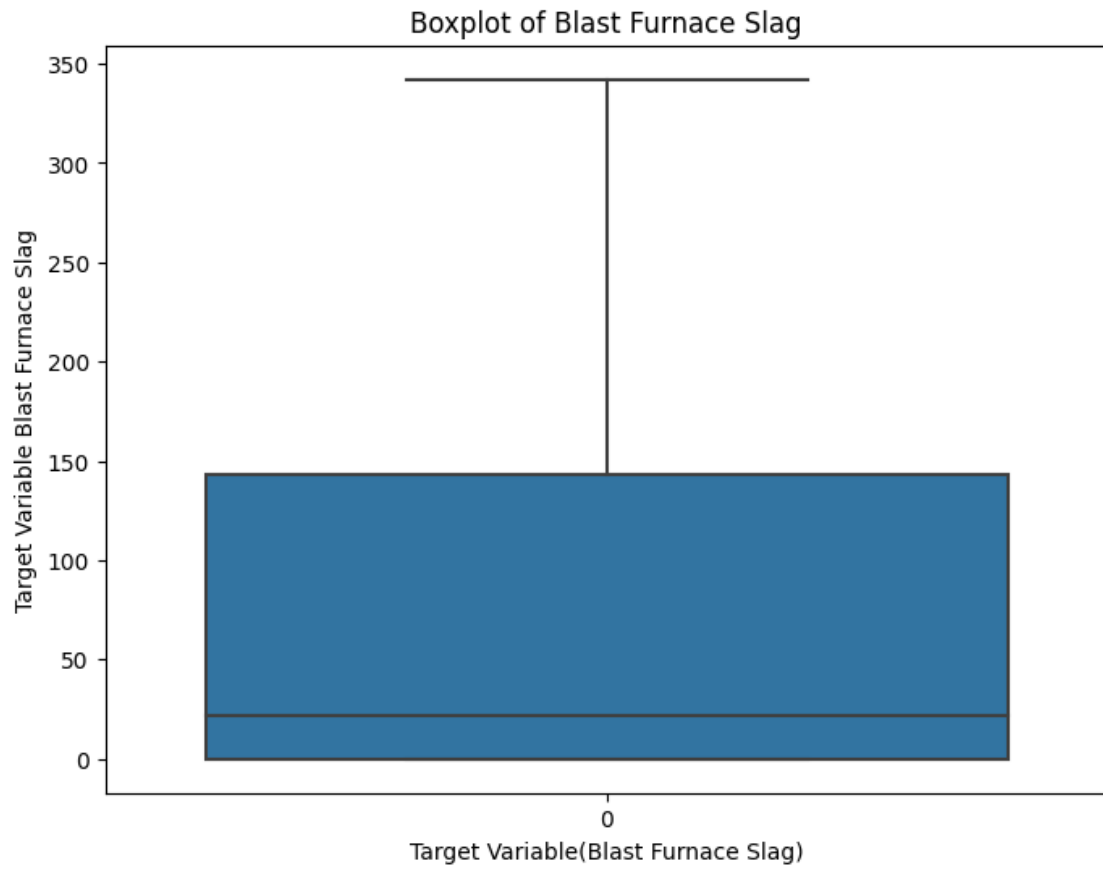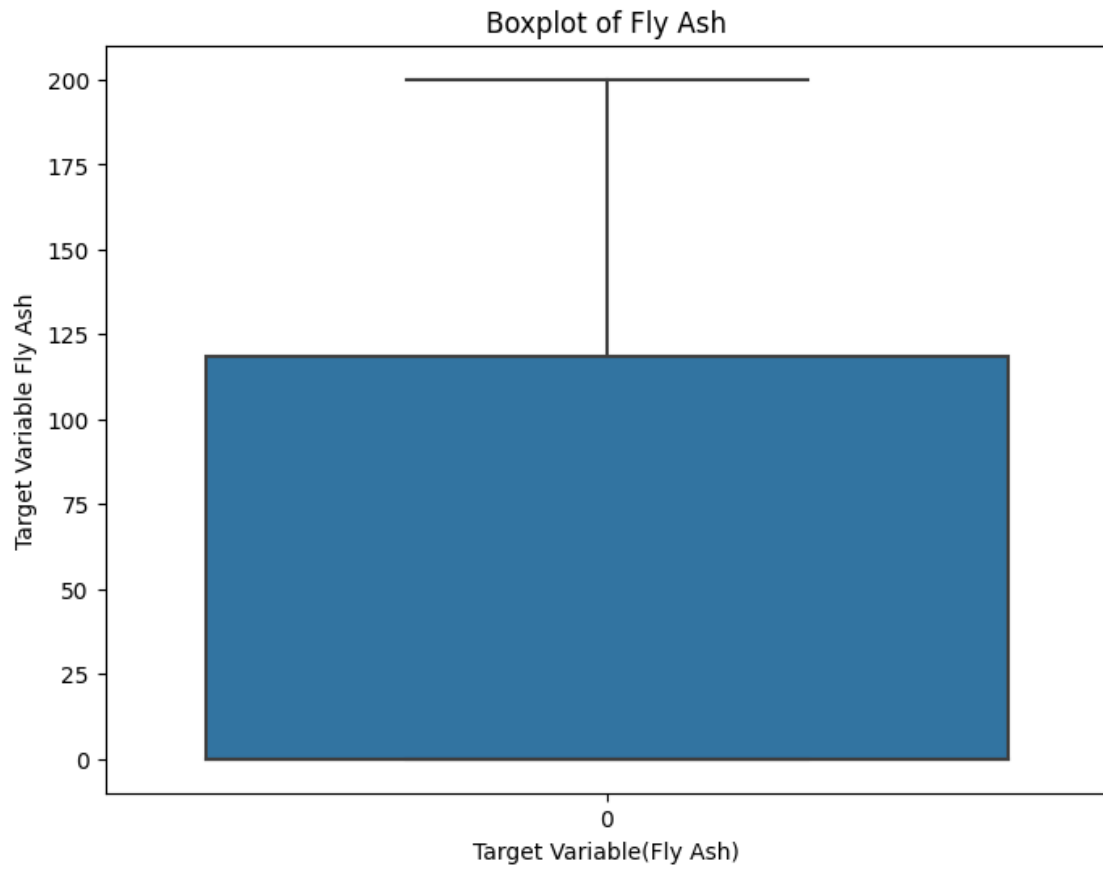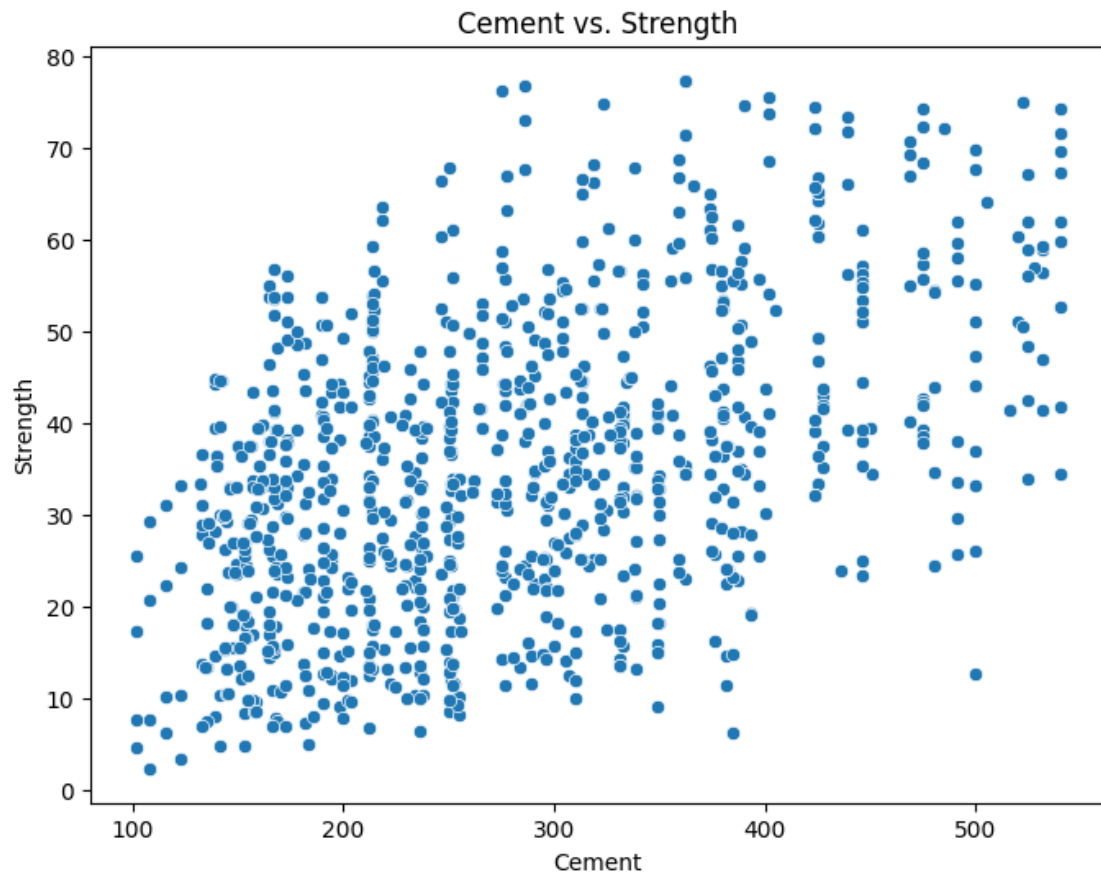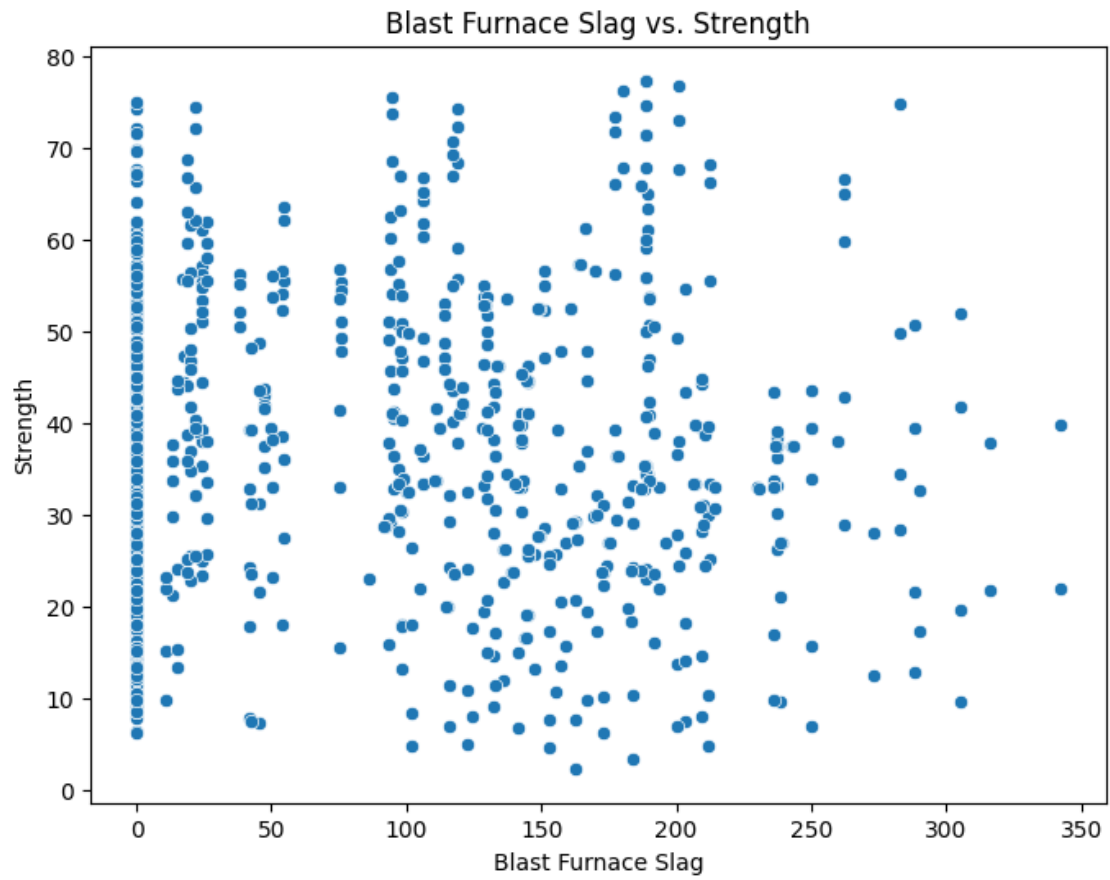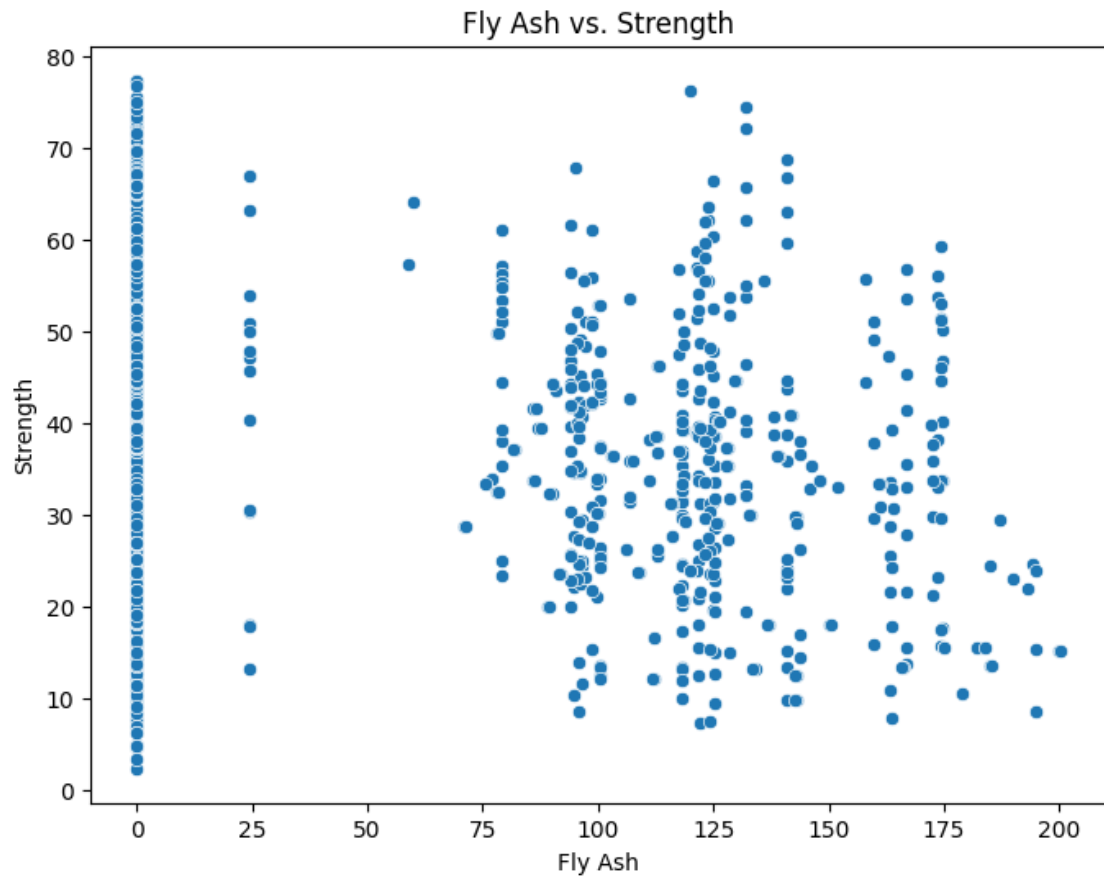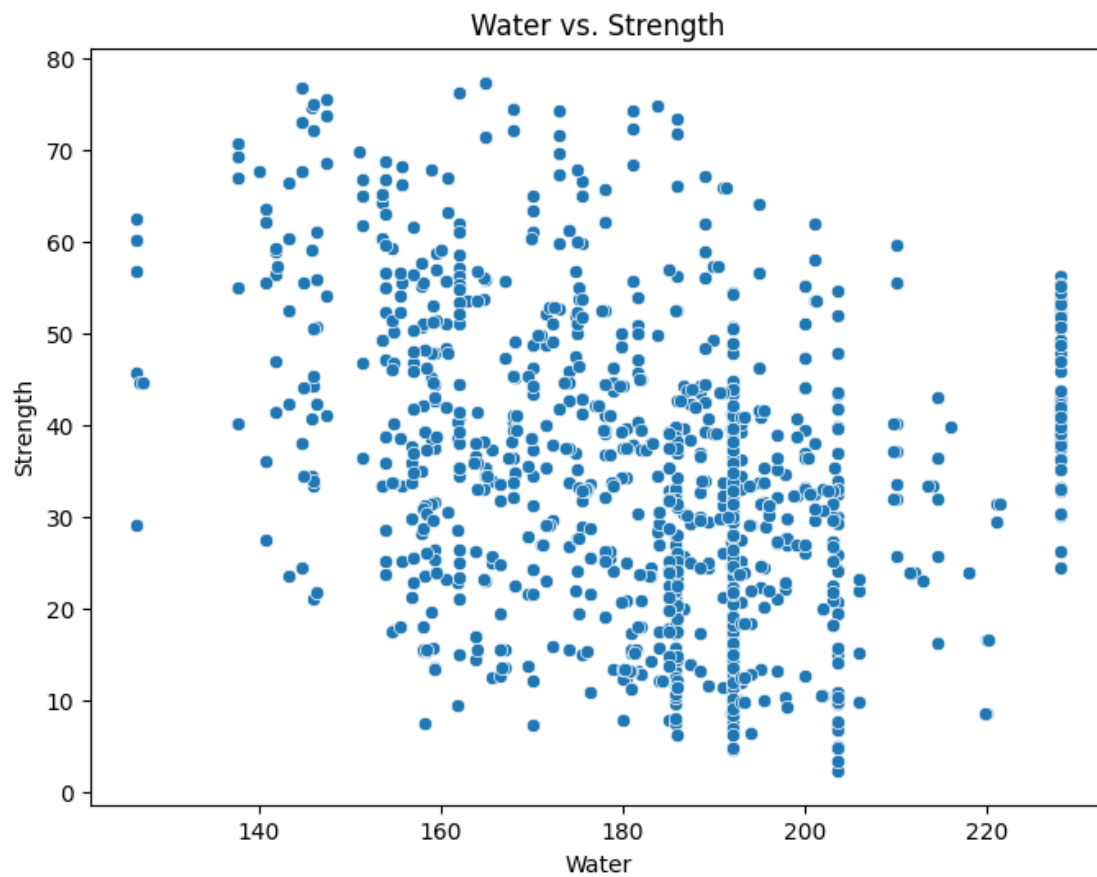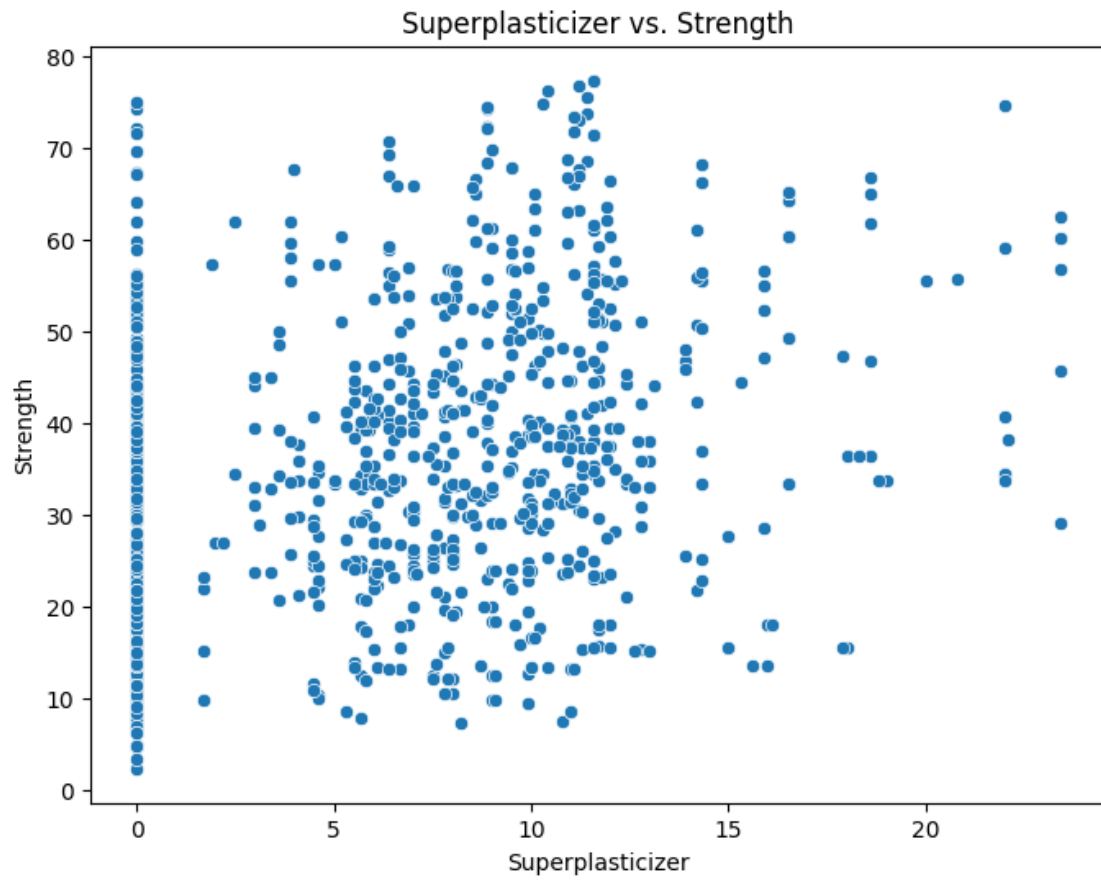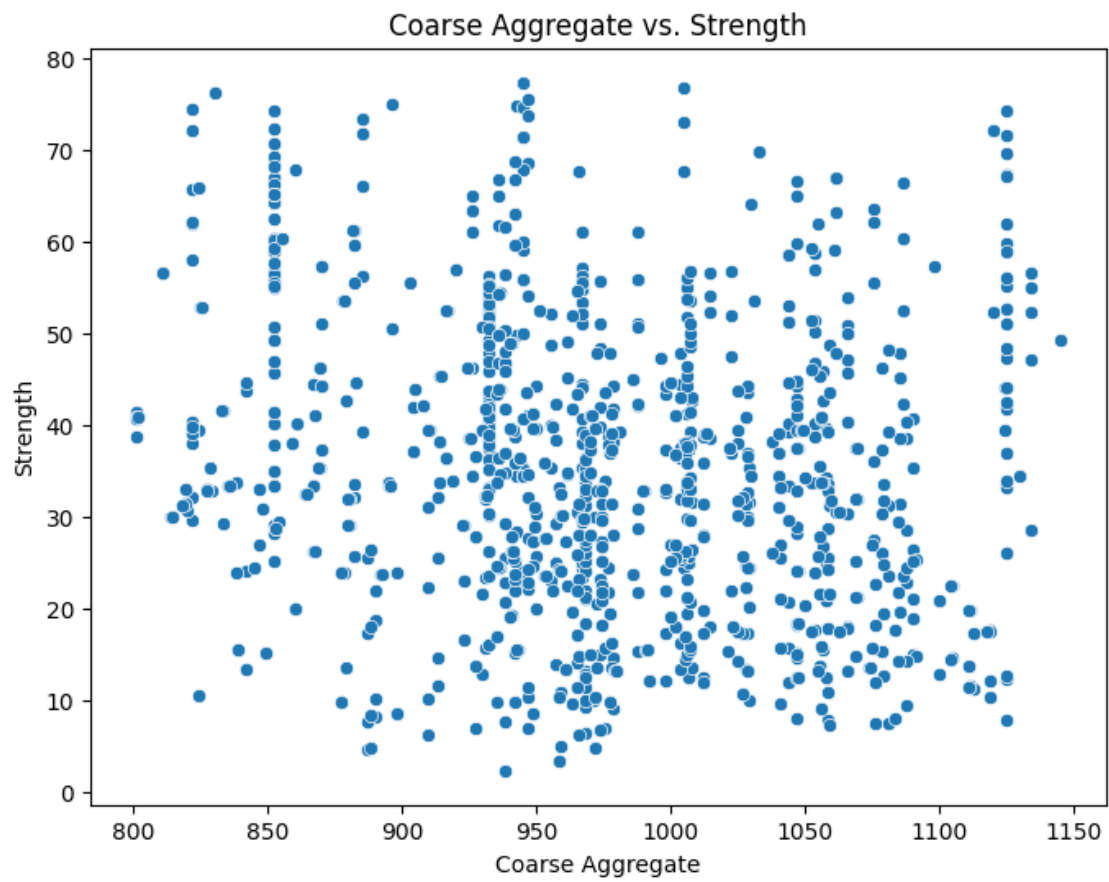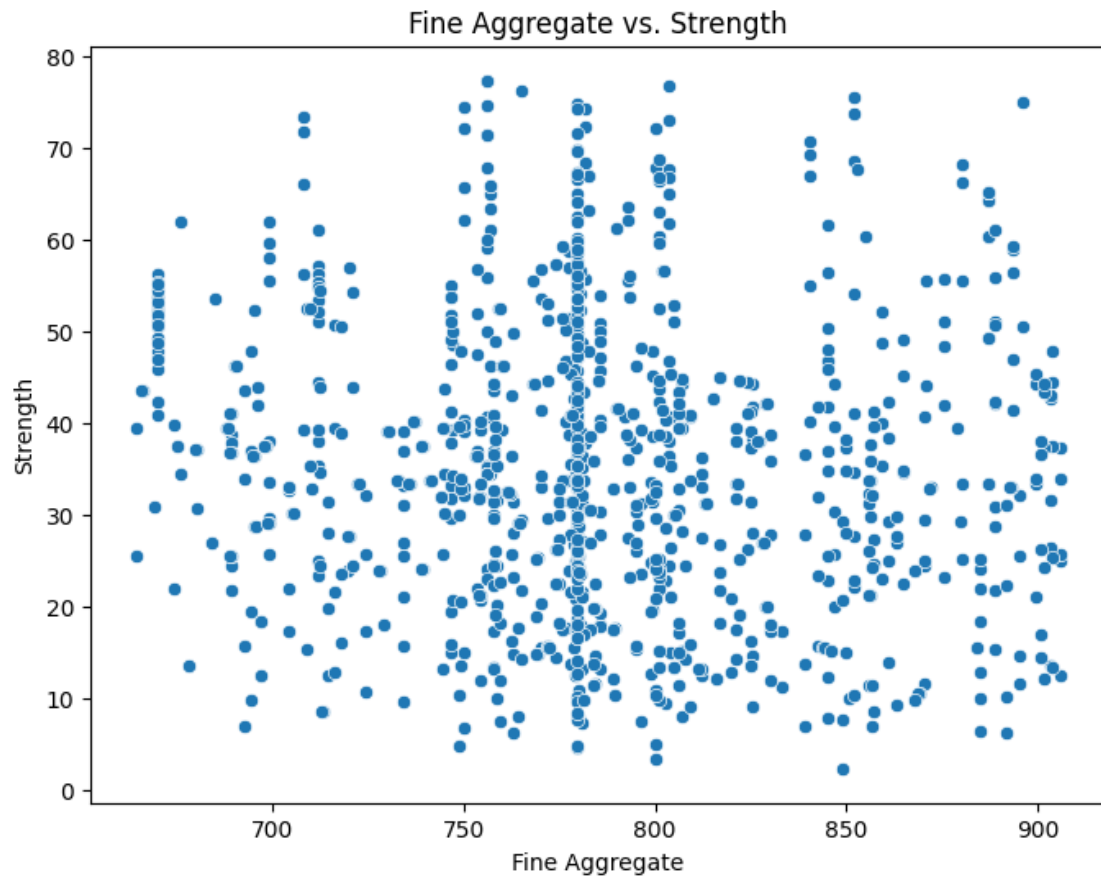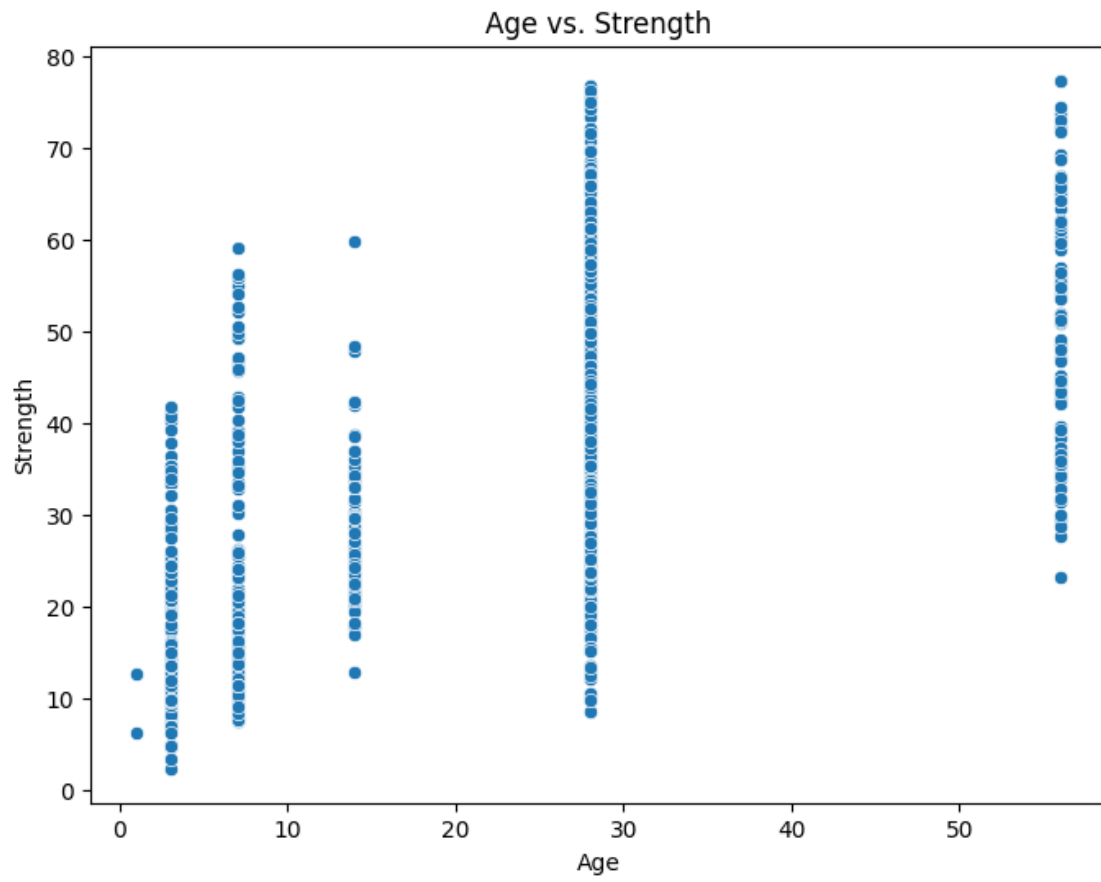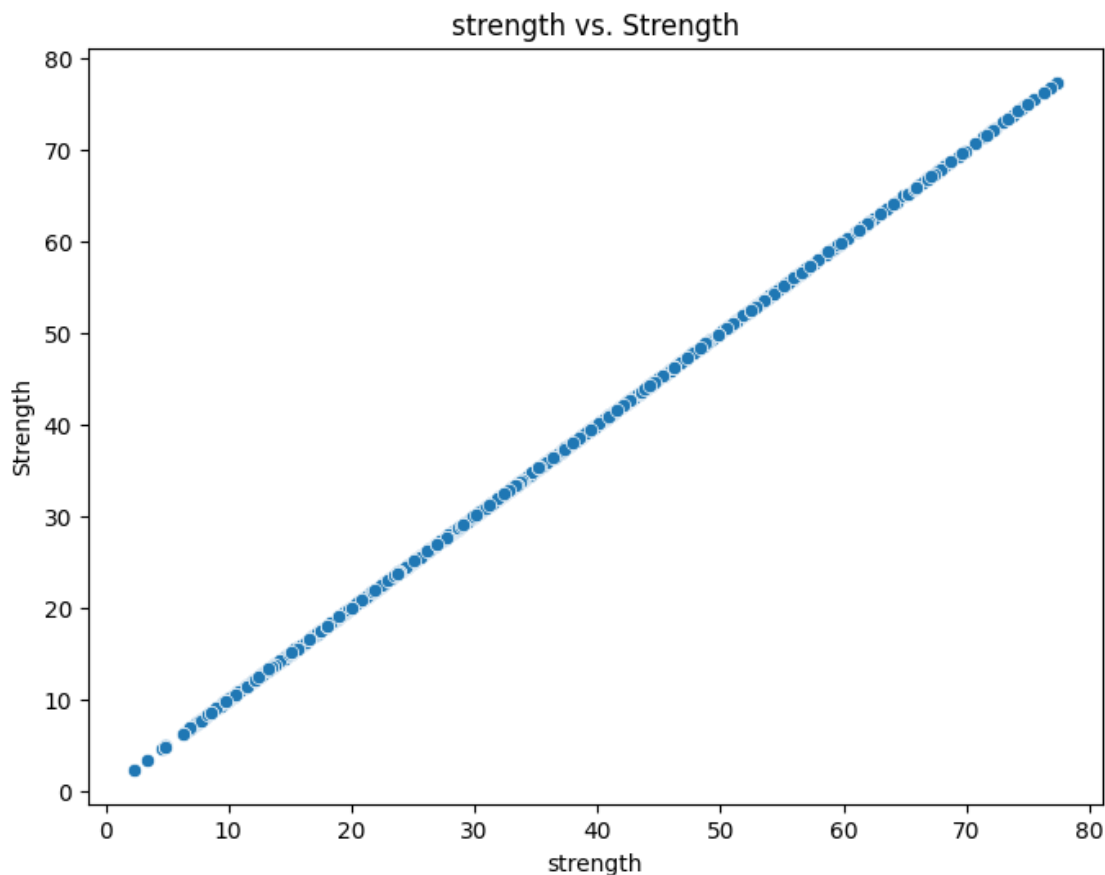
```
[19]: sns.pairplot(data)
```

/home/applehx7/anaconda3/lib/python3.11/site-packages/seaborn/_oldcore.py:1119:
FutureWarning: use_inf_as_na option is deprecated and will be removed in a
future version. Convert inf values to NaN before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
/home/applehx7/anaconda3/lib/python3.11/site-packages/seaborn/_oldcore.py:1119:
FutureWarning: use_inf_as_na option is deprecated and will be removed in a
future version. Convert inf values to NaN before operating instead.
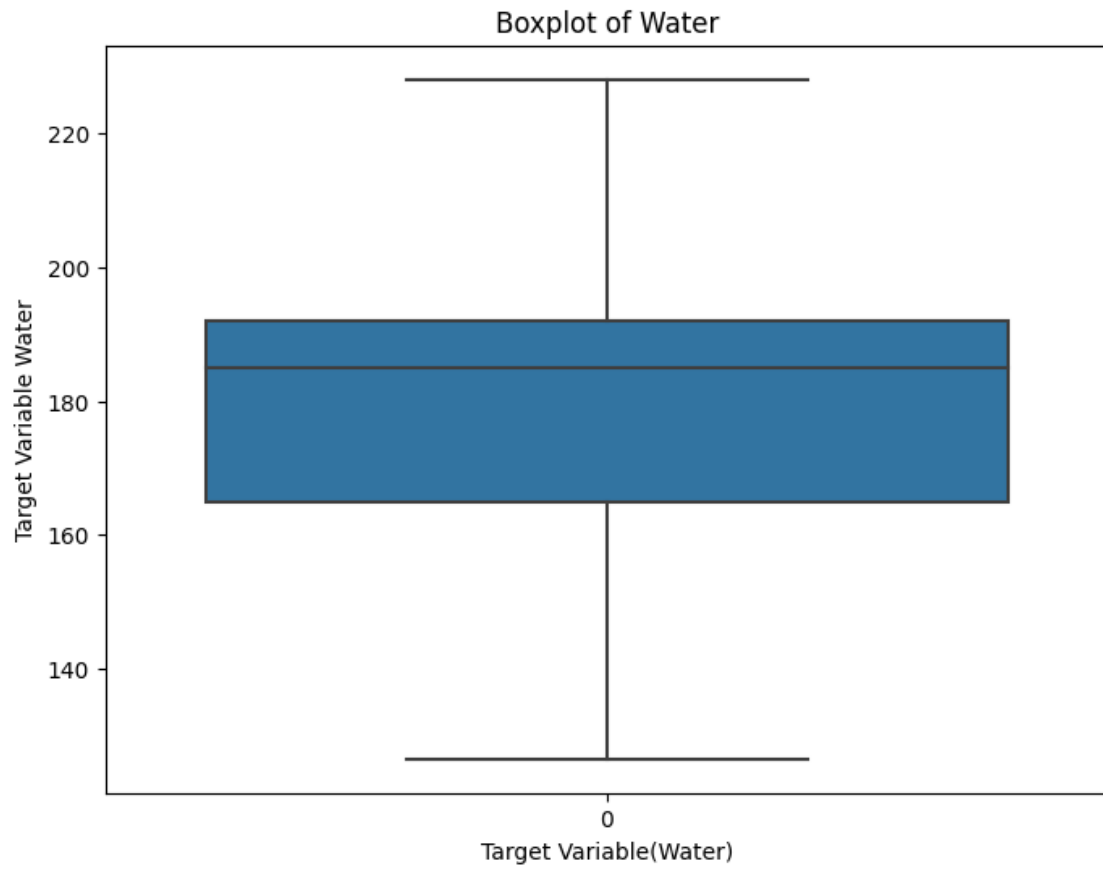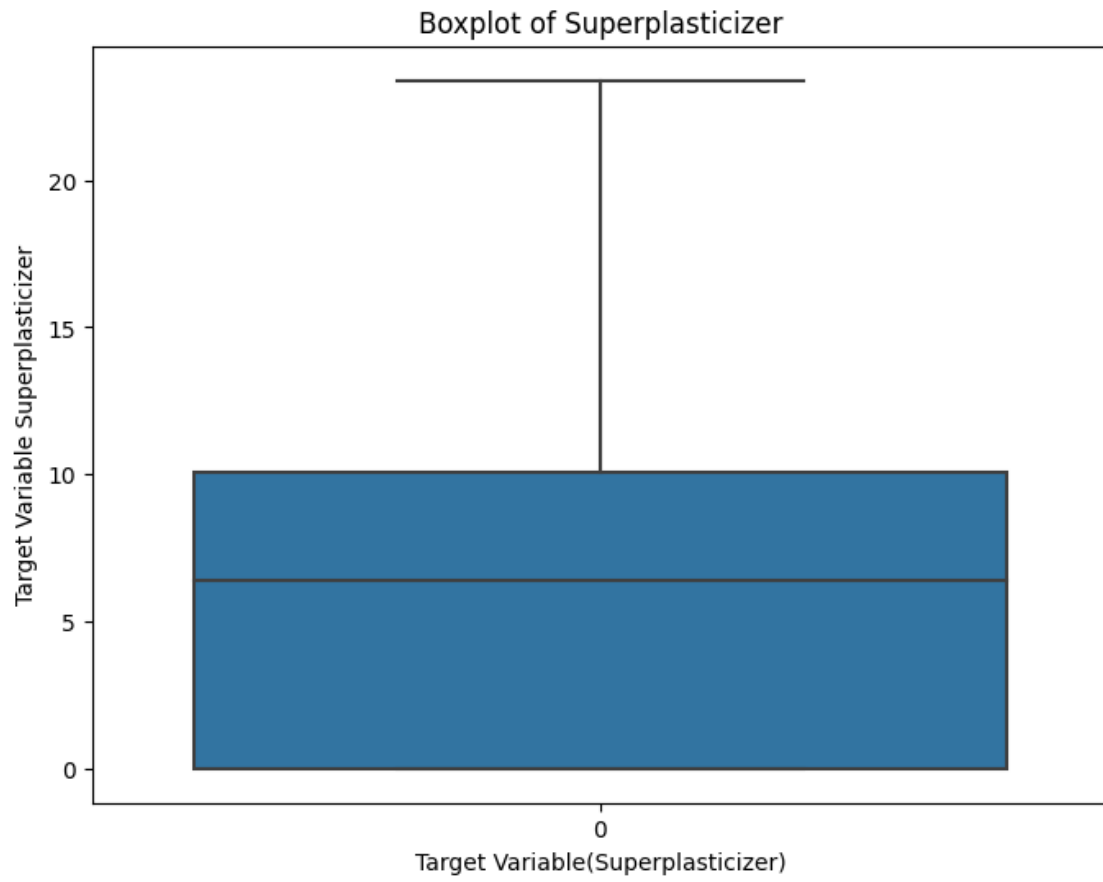 with pd.option_context('mode.use_inf_as_na', True):
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FutureWarning: use_inf_as_na option is deprecated and will be removed in a
future version. Convert inf values to NaN before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):

[19]: <seaborn.axisgrid.PairGrid at 0x7ff6cb61d490>

```
[20]: correlation_matrix = data.corr()
      plt.figure(figsize=(10, 8))
      sns.heatmap(correlation_matrix, annot=True, cmap='bone', fmt='.2f')
      plt.title('Correlation Heatmap')
      plt.show()
```

Correlation Heatmap
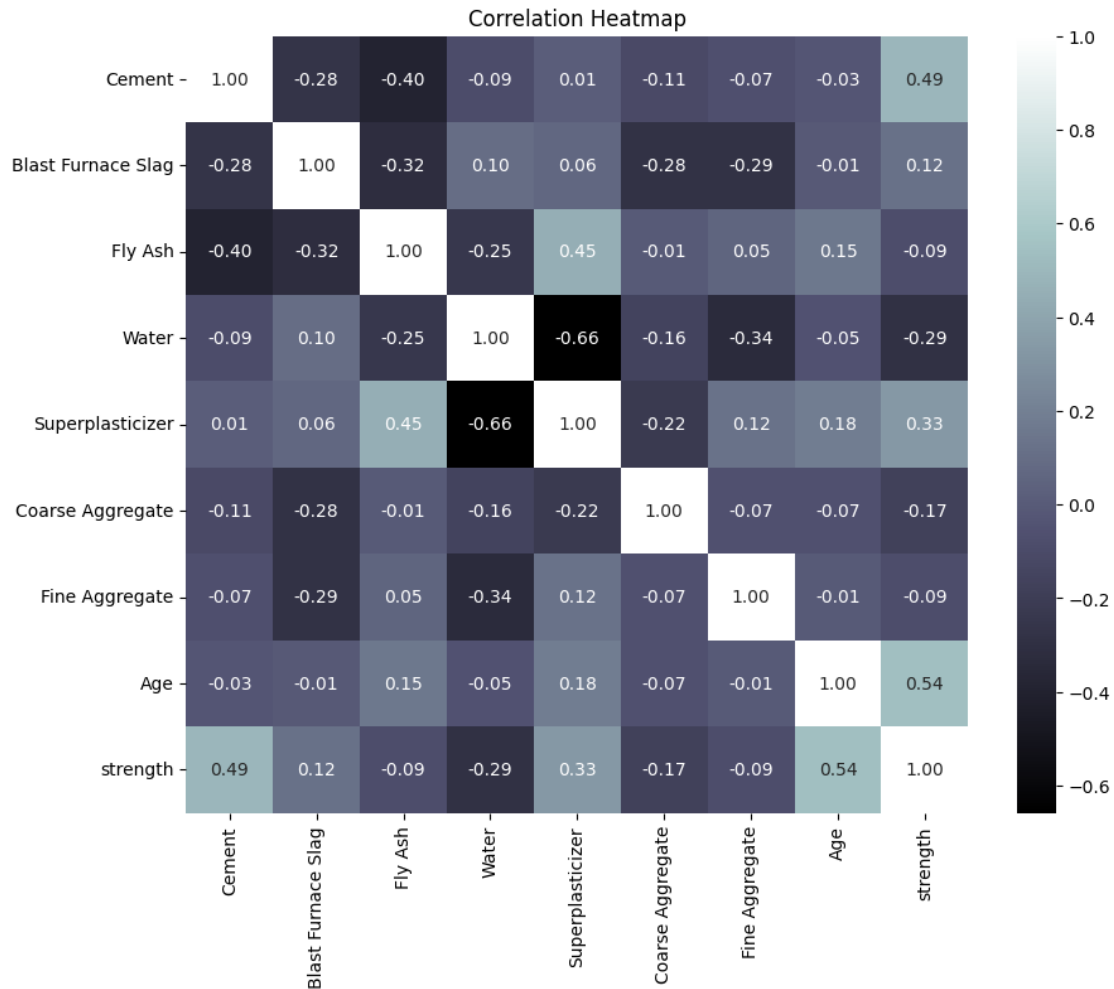
0.0.4 Scaling and Splitting

```
[21]: x = data.drop(['strength'], axis=1)
      y = pd.DataFrame(data['strength'])
```

```
[22]: X_train, X_test, Y_train, Y_test = train_test_split(x, y, test_size=.3,
      ↪random_state=42)
```

```
[23]: scaler = StandardScaler()
```

```
[24]: X_train = pd.DataFrame(scaler.fit_transform(X_train), columns=X_train.columns)
      X_test = pd.DataFrame(scaler.transform(X_test), columns=X_test.columns)
```

0.0.5 Model Selection and Training

```
[28]: models = [
          LinearRegression(),
          RandomForestRegressor(),
          xgb()
      ]
```

```
[29]: def train_md(model, X, Y, testX):
          model.fit(X, Y)
          predicted = model.predict(testX)
          model_name = type(model).__name__
          return model_name, predicted
```

```
[30]: model_inf = {}
```

```
[31]: for model in models:
          name, pred = train_md(model, X_train, Y_train, X_test)
          model_inf[name] = {'actual_Y': Y_test, 'predicted_Y': pred}
```

```
/tmp/ipykernel_36832/2794685275.py:2: DataConversionWarning: A column-vector y
was passed when a 1d array was expected. Please change the shape of y to
(n_samples,), for example using ravel().
  model.fit(X, Y)
```

0.0.6 Evaluation

```
[32]: def get_score(x, y):
          sc = {
                  'MSE' : mean_squared_error(x, y),
                  'MAE' : mean_absolute_error(x, y),
                  'R2' : r2_score(x, y),
                  'RMSE' : np.sqrt(mean_squared_error(x, y))
          }
          return sc
```

```
[33]: score = {}

      for model_name in model_inf:
          sc = get_score(model_inf[model_name]['actual_Y'],
       ↪model_inf[model_name]['predicted_Y'])
          score[model_name] = sc
```

```
[34]: for name in score:
          print("-----------*******----------")
          print(name)
          for i in score[name]:
```

```
        print(i, ":", score[name][i])
```

```
----------********----------
LinearRegression
MSE : 76.56408075141017
MAE : 6.790782891617033
R2 : 0.7094232945986152
RMSE : 8.75009032818577
----------********----------
RandomForestRegressor
MSE : 47.53329023278639
MAE : 4.947496895975295
R2 : 0.8196012185194753
RMSE : 6.8944390803593585
----------********----------
XGBRegressor
MSE : 47.21011467270518
MAE : 4.7518051358565545
R2 : 0.8208277373856725
RMSE : 6.8709616992605325
```

0.0.7 Feature Importance

```
[35]: rf = RandomForestRegressor()
      rf.fit(X_train, Y_train)
      feature_importances_rf = rf.feature_importances_

      indices_rf = np.argsort(feature_importances_rf)[::-1]

      plt.figure(figsize=(10, 6))
      plt.title("Feature Importances (RANDOM FOREST)")
      plt.bar(range(X_train.shape[1]), feature_importances_rf[indices_rf],␣
       ↪align="center")
      plt.xticks(range(X_train.shape[1]), X_train.columns[indices_rf], rotation=90)
      plt.xlim([-1, X_train.shape[1]])
      plt.tight_layout()
      plt.show()
```

```
/tmp/ipykernel_36832/1490296704.py:2: DataConversionWarning: A column-vector y
was passed when a 1d array was expected. Please change the shape of y to
(n_samples,), for example using ravel().
  rf.fit(X_train, Y_train)
```

Feature Importances (RANDOM FOREST)
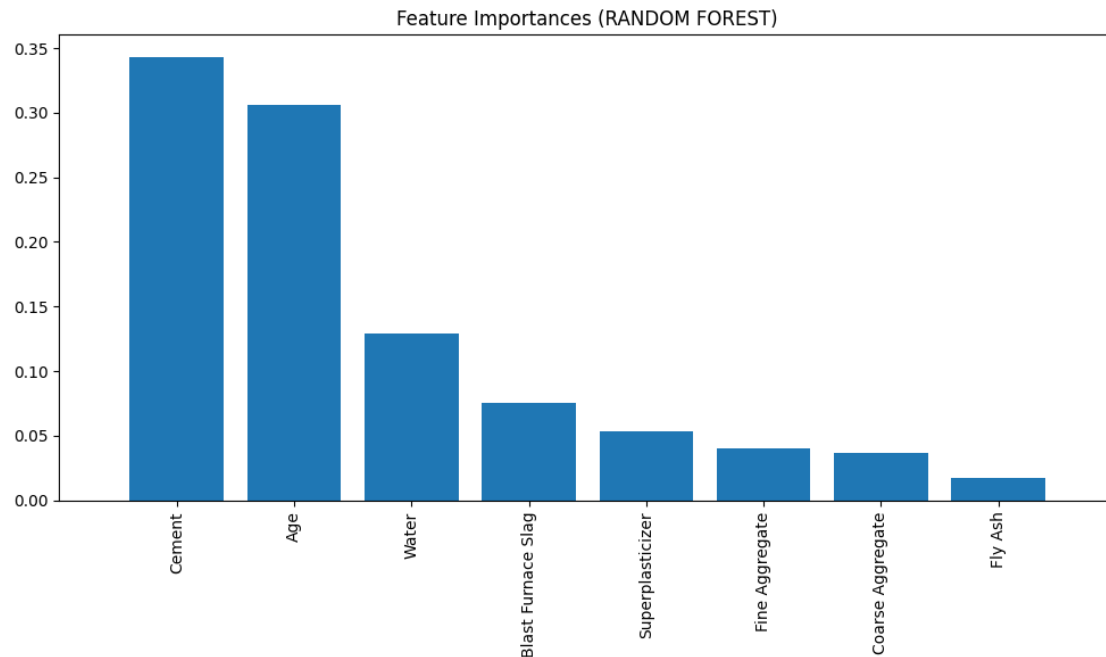
```
[37]: xgboost = xgb()
      xgboost.fit(X_train, Y_train)
      feature_importances_xgb = xgboost.feature_importances_
      indices_xgb = np.argsort(feature_importances_xgb)[::-1]

      plt.figure(figsize=(10, 6))
      plt.title("XGBoost Feature Importances")
      plt.bar(range(X_train.shape[1]), feature_importances_xgb[indices_xgb],␣
       ↪align="center")
      plt.xticks(range(X_train.shape[1]), X_train.columns[indices_xgb], rotation=90)
      plt.xlim([-1, X_train.shape[1]])
      plt.tight_layout()
      plt.show()
```

XGBoost Feature Importances

[ ]:
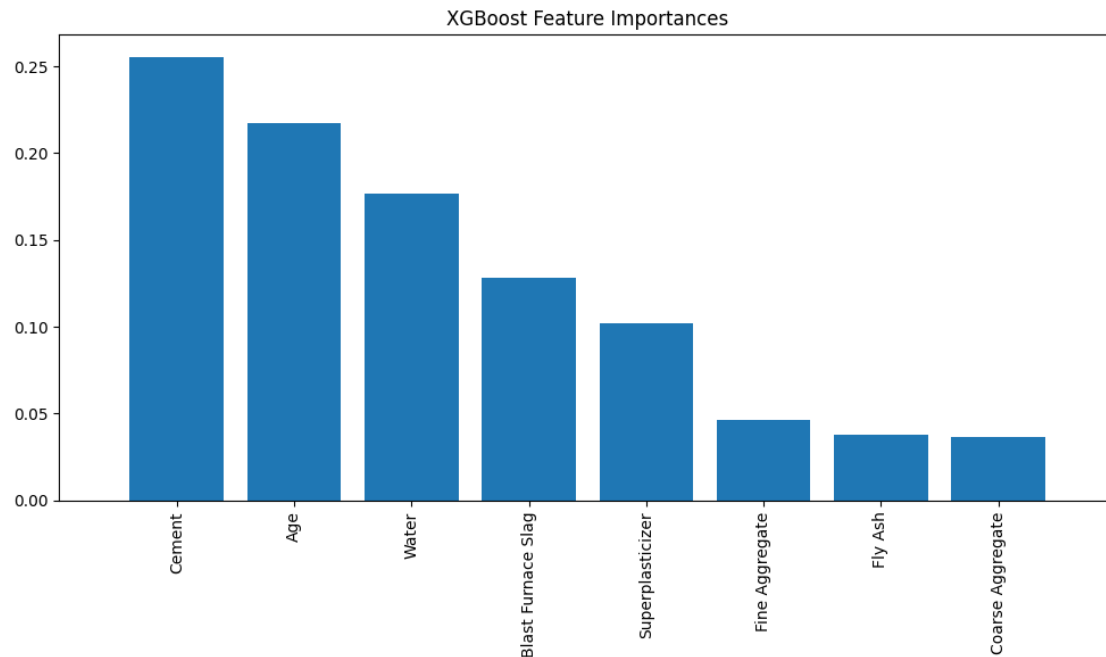
0.0.8 HyperParameter Tuning

```
[39]: models = {
          LinearRegression(): {
              'params': {
                  'fit_intercept': [True, False],
                  'copy_X': [True, False],
                  'n_jobs': [1, 2, 3],
                  'positive': [True, False]
              }
          },
          RandomForestRegressor(): {
              'params': {
                  'n_estimators': [20, 50, 100, 200],
                  'criterion': ['squared_error', 'absolute_error'],
                  'min_samples_leaf': [1, 2],
                  'max_features': ['sqrt', 'log2']
              }
          },
          xgb(): {
              'params': {
                  'learning_rate': [0.1, 0.01, 0.001, 2],
                  'n_estimators': [20, 50, 100, 200],
```

```
            'criterion': ['friedman_mse', 'squared_error'],
            'min_samples_leaf': [1, 2]
        }
    },
}
```

[40]: ```
model_info = {}
```

[41]: ```
for model in models:
    clf = RandomizedSearchCV(model,␣
 ↪param_distributions=models[model]['params'], random_state=0, n_iter=50)
    clf.fit(X_train, Y_train)
    model_info[type(model).__name__] = {'Best Score': clf.best_score_,␣
 ↪'BestFittedModel': clf.best_estimator_}
```

/home/applehx7/anaconda3/lib/python3.11/site-
packages/sklearn/model_selection/_search.py:305: UserWarning: The total space of
parameters 24 is smaller than n_iter=50. Running 24 iterations. For exhaustive
searches, use GridSearchCV.
  warnings.warn(
/home/applehx7/anaconda3/lib/python3.11/site-
packages/sklearn/model_selection/_search.py:305: UserWarning: The total space of
parameters 32 is smaller than n_iter=50. Running 32 iterations. For exhaustive
searches, use GridSearchCV.
  warnings.warn(
/home/applehx7/anaconda3/lib/python3.11/site-
packages/sklearn/model_selection/_validation.py:686: DataConversionWarning: A
column-vector y was passed when a 1d array was expected. Please change the shape
of y to (n_samples,), for example using ravel().
  estimator.fit(X_train, y_train, **fit_params)
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```

[42]:
```python
model_info
```

[42]:
```
{'LinearRegression': {'Best Score': 0.6643038573087645,
  'BestFittedModel': LinearRegression(n_jobs=1)},
 'RandomForestRegressor': {'Best Score': 0.8040859020615324,
  'BestFittedModel': RandomForestRegressor(max_features='log2')},
 'XGBRegressor': {'Best Score': 0.808336466556104,
  'BestFittedModel': XGBRegressor(base_score=None, booster=None, callbacks=None,
              colsample_bylevel=None, colsample_bynode=None,
              colsample_bytree=None, criterion='squared_error', device=None,
              early_stopping_rounds=None, enable_categorical=False,
              eval_metric=None, feature_types=None, gamma=None,
 grow_policy=None,
              importance_type=None, interaction_constraints=None,
              learning_rate=0.1, max_bin=None, max_cat_threshold=None,
              max_cat_to_onehot=None, max_delta_step=None, max_depth=None,
              max_leaves=None, min_child_weight=None, min_samples_leaf=1,
              missing=nan, monotone_constraints=None, multi_strategy=None,
              n_estimators=50, n_jobs=None, …)}}
```

0.0.9 Evaluation Metrics:

```python
[43]: for model_name in model_info:
          actual_y = Y_test
          pred_y = model_info[model_name]['BestFittedModel'].predict(X_test)

          mse = mean_squared_error(actual_y, pred_y)
          mae = mean_absolute_error(actual_y, pred_y)
          r2score = r2_score(actual_y, pred_y)
          rmse = np.sqrt(mse)

          print(f"----------*** {model_name} ***----------")
          print("Mean Squared Error: ", mse)
          print("Mean Absolute Error: ", mae)
          print("R2 Score: ", r2score)
          print("Root Mean Squared Error", rmse)
          print("")
```

```
----------*** LinearRegression ***----------
Mean Squared Error:  76.56408075141017
Mean Absolute Error:  6.790782891617033
R2 Score:  0.7094232945986152
Root Mean Squared Error 8.75009032818577

----------*** RandomForestRegressor ***----------
Mean Squared Error:  42.750727139238265
Mean Absolute Error:  4.768612781553893
R2 Score:  0.8377520460806339
Root Mean Squared Error 6.538404020801885

----------*** XGBRegressor ***----------
Mean Squared Error:  45.15558617635081
Mean Absolute Error:  4.742664722887058
R2 Score:  0.8286251028834999
Root Mean Squared Error 6.7197906348598995
```

0.1 Comparative Analysis:

1. Performance Evaluation Metrics:
   - Use evaluation metrics such as Mean Absolute Error (MAE), Mean Squared Error (MSE), Root Mean Squared Error (RMSE), and R-squared (R2) score.
   - Compute these metrics for each model using the same testing dataset.
   - Analyze which model performs better based on these metrics. For instance, lower values of MAE, MSE, and RMSE indicate better predictive performance, while higher R2 scores signify a better fit of the model.

2. Strengths of Models:

- Discuss the strengths of each model in the context of concrete strength prediction:
- Linear Regression: Simplicity, easy interpretability, works well with linear relationships in data.
- Random Forest Regressor: Handles nonlinear relationships, robust to outliers, less prone to overfitting.
- Gradient Boosting Regressor (XGBoost): Better predictive accuracy, handles complex relationships, feature importance insights.

3. Limitations of Models:

- Highlight the limitations of each model:
- Linear Regression: Assumption of linear relationships might not hold in real-world scenarios, sensitive to outliers.
- Random Forest Regressor: Complexity, may overfit with a large number of trees, less interpretable compared to simpler models.
- Gradient Boosting Regressor (XGBoost): Computationally expensive, tuning parameters might be tricky, potential overfitting with improper hyperparameters.

4. Model Interpretability:

- Discuss how easy or difficult it is to interpret and explain the predictions of each model. Linear Regression offers straightforward interpretation, while tree-based models like Random Forest and Gradient Boosting might provide insights into feature importance but are more complex to interpret.

5. Scalability and Efficiency:

- Consider the scalability and efficiency of models when working with larger datasets. Linear Regression is usually more scalable, whereas ensemble models like Random Forest and Gradient Boosting might require more computational resources.

6. Handling of Nonlinear Relationships:

- Highlight the capability of models to capture nonlinear relationships in concrete strength prediction. Tree-based models like Random Forest and Gradient Boosting inherently handle nonlinear relationships better than Linear Regression.

7. Robustness to Data Variation:

- Discuss how each model performs in the presence of noisy or incomplete data. Robust models like Random Forest and Gradient Boosting might handle such variations better than Linear Regression.

[ ]: