# u2003961-assignment-1

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# 1 Assignment 1 - Concrete Data

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## 1.1 Download the Data

[76]:
```
from pathlib import Path
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

concrete = pd.read_excel('Concrete_Data.xls')
```

## 1.2 A Quick Look at the Data Structure

[77]:
```
concrete.head()
```

[77]:
```
   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)  \
0                                              676.0         28
1                                              676.0         28
2                                              594.0        270
3                                              594.0        365
4                                              825.5        360

   Concrete compressive strength(MPa, megapascals)
0                                        79.986111
1                                        61.887366
2                                        40.269535
3                                        41.052780
4                                        44.296075
```

[78]:

```
#change column name
concrete.columns = ['cement', 'slag', 'ash', 'water', 'superplastic',␣
 ↪'coarseagg', 'fineagg', 'age', 'strength']
```

[79]:

```
concrete.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1030 entries, 0 to 1029
Data columns (total 9 columns):
 #   Column        Non-Null Count  Dtype
```

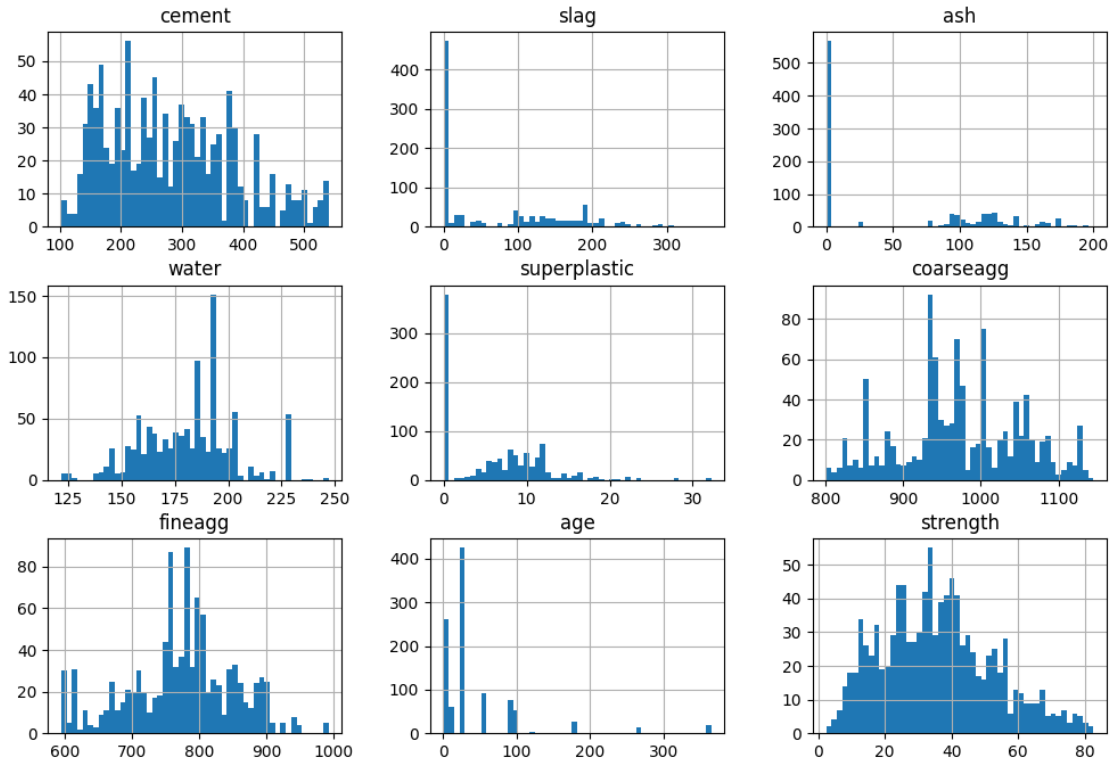
```
---  ------        --------------  -----
 0   cement        1030 non-null   float64
 1   slag          1030 non-null   float64
 2   ash           1030 non-null   float64
 3   water         1030 non-null   float64
 4   superplastic  1030 non-null   float64
 5   coarseagg     1030 non-null   float64
 6   fineagg       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
```

[80]:
```
concrete.describe()
```

[80]:
```
            cement         slag          ash        water  superplastic  \
count  1030.000000  1030.000000  1030.000000  1030.000000   1030.000000
mean    281.165631    73.895485    54.187136   181.566359      6.203112
std     104.507142    86.279104    63.996469    21.355567      5.973492
min     102.000000     0.000000     0.000000   121.750000      0.000000
25%     192.375000     0.000000     0.000000   164.900000      0.000000
50%     272.900000    22.000000     0.000000   185.000000      6.350000
75%     350.000000   142.950000   118.270000   192.000000     10.160000
max     540.000000   359.400000   200.100000   247.000000     32.200000

         coarseagg      fineagg          age     strength
count  1030.000000  1030.000000  1030.000000  1030.000000
mean    972.918592   773.578883    45.662136    35.817836
std      77.753818    80.175427    63.169912    16.705679
min     801.000000   594.000000     1.000000     2.331808
25%     932.000000   730.950000     7.000000    23.707115
50%     968.000000   779.510000    28.000000    34.442774
75%    1029.400000   824.000000    56.000000    46.136287
max    1145.000000   992.600000   365.000000    82.599225
```

[81]:
```
concrete.hist(bins=50, figsize=(12, 8))
plt.show()
```




[82]:
```
concrete.isnull().sum()
```

[82]:
```
cement          0
slag            0
ash             0
water           0
superplastic    0
coarseagg       0
fineagg         0
age             0
strength        0
dtype: int64
```

### 1.3 Create a Test Set

[83]:
```
concrete["strengthy"] = pd.cut(concrete["strength"],
bins=[0, 20.0, 40.0, 60.0, np.inf],
labels=[1, 2, 3, 4])

from sklearn.model_selection import train_test_split
strat_train_set, strat_test_set = train_test_split(
concrete, test_size=0.15, stratify=concrete["strengthy"], random_state=42)
```

```python
for set_ in (strat_train_set, strat_test_set):
    set_.drop("strengthy", axis=1, inplace=True)
```

[84]:
```python
strat_test_set.head()
```

[84]:
```
     cement   slag     ash   water  superplastic  coarseagg  fineagg  age  \
666  192.00  288.0    0.00  192.00          0.00      929.8    716.1    3
628  200.00    0.0    0.00  180.00          0.00     1125.0    845.0   28
107  323.70  282.8    0.00  183.80         10.30      942.7    659.9    7
285  181.38    0.0  167.01  169.59          7.56     1055.6    777.8   14
718  122.60  183.9    0.00  203.50          0.00      958.2    800.1    7

      strength
666  12.788401
628  12.245094
107  49.800851
285  21.601283
718  10.354551
```

## 1.4 Explore and Visualise the Data to Gain Insights

### 1.4.1 Make a copy of training set for data exploration

[85]:
```python
concrete = strat_train_set.copy()
```

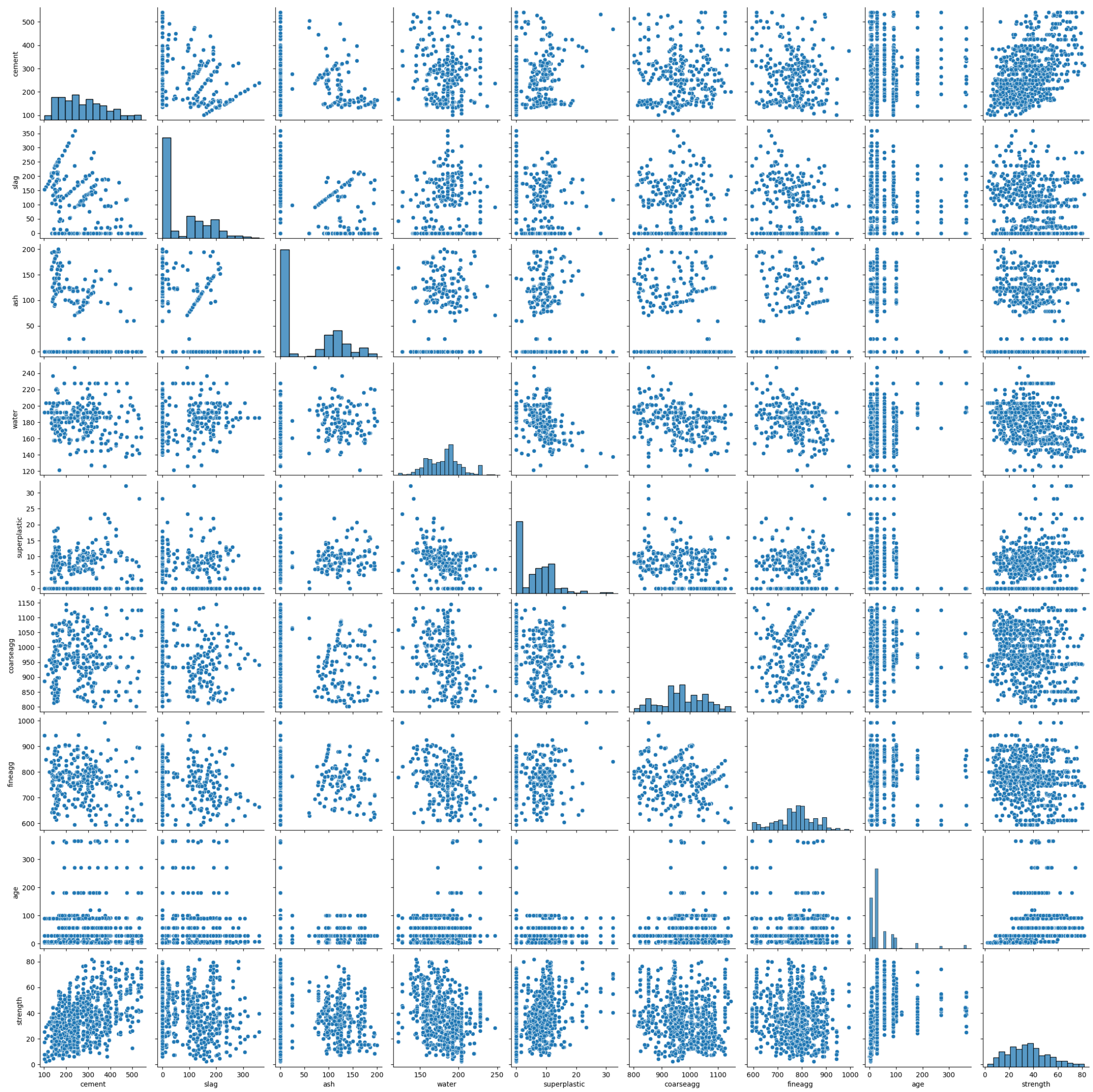
[86]:
```python
concrete.head()
```

[86]:
```
     cement    slag     ash   water  superplastic  coarseagg  fineagg  age  \
362  218.23   54.64  123.78  140.75         11.91     1075.7   792.67   56
233  213.72   98.05   24.51  181.71          6.86     1065.8   785.38  100
289  182.04   45.21  121.97  170.21          8.19     1059.4   780.65    3
737  238.00    0.00    0.00  186.00          0.00     1119.0   789.00   28
139  374.00  189.20    0.00  170.10         10.10      926.1   756.70   56

      strength
362  61.990787
233  53.903234
289   7.315340
737  17.540269
139  63.397318
```

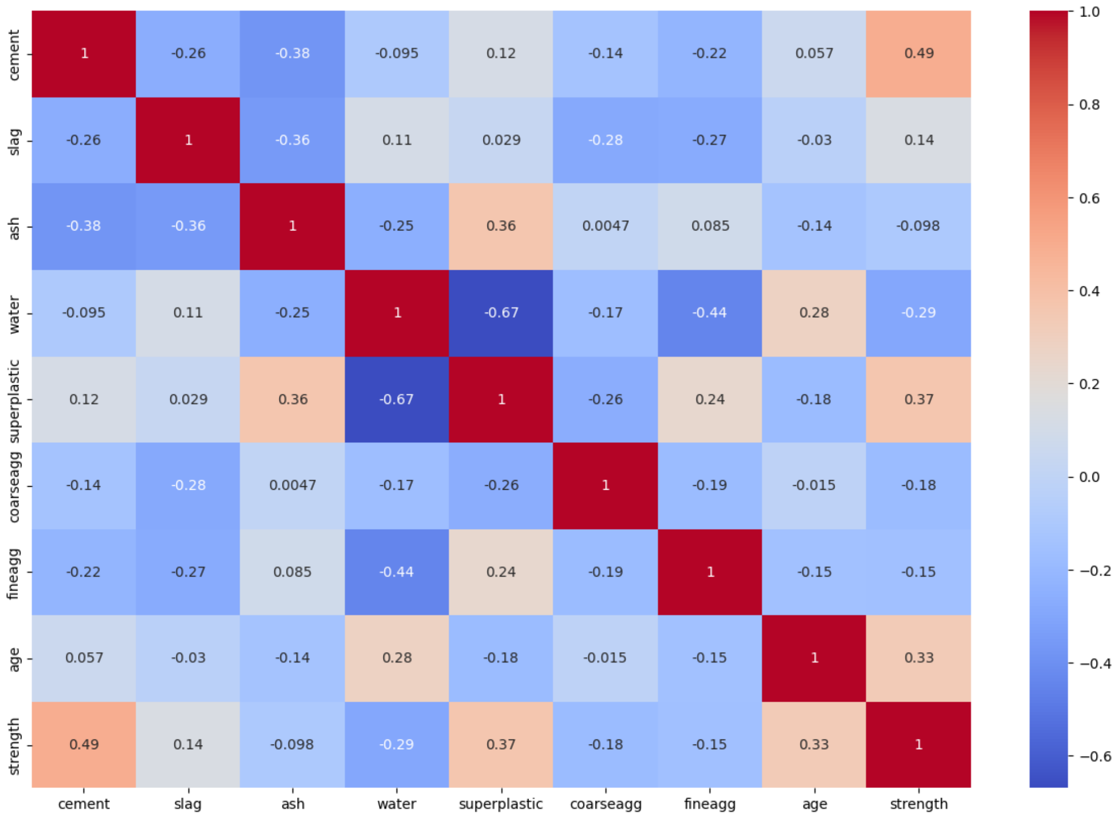
### 1.4.2 Look for correlation

[87]:
```
import seaborn as sns
sns.pairplot(concrete)
plt.show()
```




[88]:
```
corr_matrix = concrete.corr(numeric_only=True)
corr_matrix["strength"].sort_values(ascending=False)

plt.figure(figsize=(15, 10))
sns.heatmap(corr_matrix, annot=True, cmap='coolwarm')
plt.show()
```

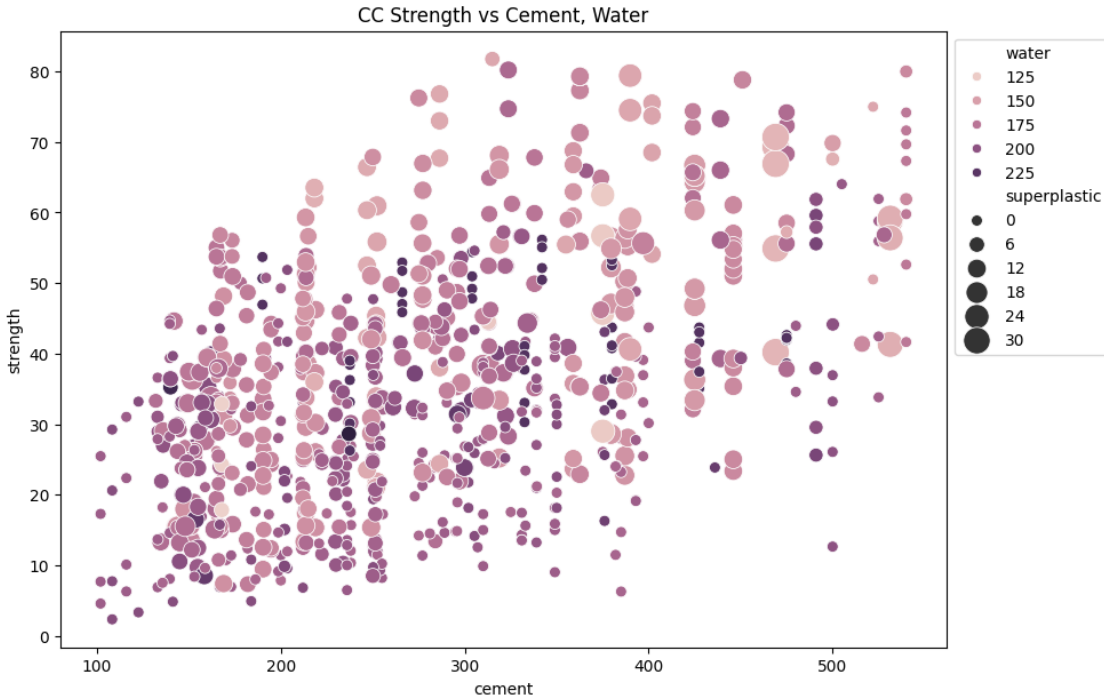



### 1.4.3 Look into more details on the median income vs median house value

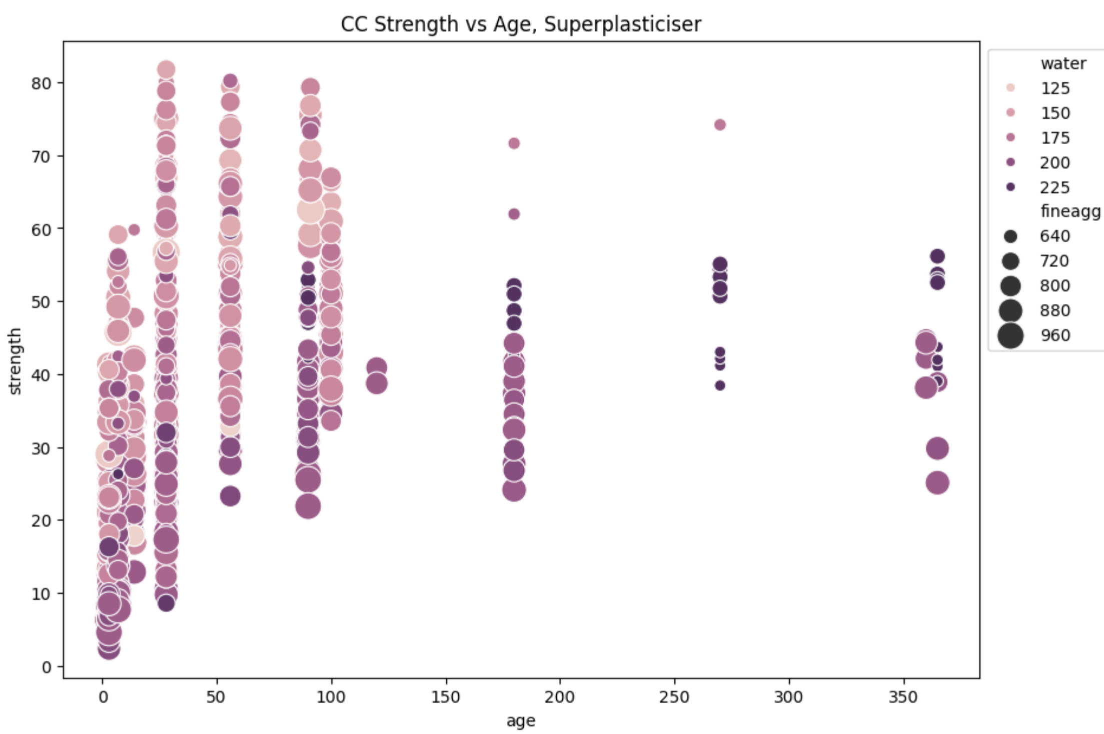
[89]:

```
fig, ax = plt.subplots(figsize=(10,7))
sns.scatterplot(y="strength", x="cement", hue="water", size= "superplastic",
                data=concrete, ax=ax, sizes=(50, 300))
ax.set_title("CC Strength vs Cement, Water")
ax.legend(loc="upper left", bbox_to_anchor=(1,1))
plt.show()

fig, ax = plt.subplots(figsize=(10,7))
sns.scatterplot(y="strength", x="age", hue="water", size = "fineagg",
                data=concrete, ax=ax, sizes=(50, 300))
ax.set_title("CC Strength vs Age, Superplasticiser")
ax.legend(loc="upper left", bbox_to_anchor=(1,1))
```




[89]: <matplotlib.legend.Legend at 0x1e7b5290440>



CC Strength increases, water decreases, superplasticzer increases

CC Srength increases, age decreases

age increases, water needed is increases to get more cc strength

#### 1.4.4 Experiment with Attribute Combinations

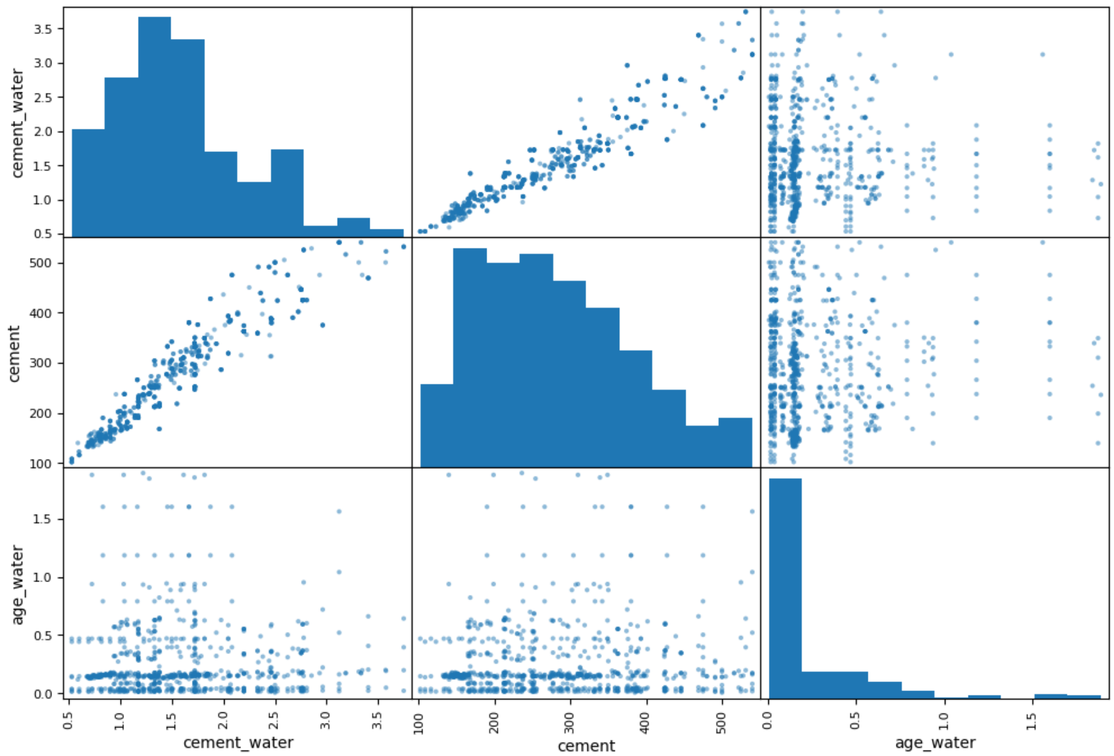
[90]:
```
concrete["cement_water"] = concrete["cement"] / concrete["water"]
concrete["superplastic_water"] = concrete["superplastic"] / concrete["water"]
concrete["age_water"] = concrete["age"] / concrete["water"]
concrete["fineagg_water"] = concrete["fineagg"] / concrete["water"]
```

#### 1.4.5 Compare with previous correlation matrix

[91]:
```
corr_matrix = concrete.corr(numeric_only=True)
corr_matrix["strength"].sort_values(ascending=False)
```

[91]:
```
strength              1.000000
cement_water          0.554364
cement                0.493710
age_water             0.389306
superplastic_water    0.378130
superplastic          0.367267
age                   0.329200
fineagg_water         0.137734
slag                  0.135618
ash                  -0.098393
fineagg              -0.154906
coarseagg            -0.183479
water                -0.294820
Name: strength, dtype: float64
```

[92]:
```
from pandas.plotting import scatter_matrix
attributes = [ "cement_water", "cement", "age_water"]
scatter_matrix(concrete[attributes], figsize=(12, 8))
plt.show()
```




## 1.5 Prepare the Data for Machine Learning Algorithms

### 1.5.1 Split the features and target - get the target into its own dataframe

[93]:
```
concrete = strat_train_set.drop("strength", axis=1)
concrete_labels = strat_train_set["strength"].copy()
```

[94]:
```
concrete.head()
```

[94]:

| | cement | slag | ash | water | superplastic | coarseagg | fineagg | age |
|---|---|---|---|---|---|---|---|---|
| 362 | 218.23 | 54.64 | 123.78 | 140.75 | 11.91 | 1075.7 | 792.67 | 56 |
| 233 | 213.72 | 98.05 | 24.51 | 181.71 | 6.86 | 1065.8 | 785.38 | 100 |
| 289 | 182.04 | 45.21 | 121.97 | 170.21 | 8.19 | 1059.4 | 780.65 | 3 |
| 737 | 238.00 | 0.00 | 0.00 | 186.00 | 0.00 | 1119.0 | 789.00 | 28 |
| 139 | 374.00 | 189.20 | 0.00 | 170.10 | 10.10 | 926.1 | 756.70 | 56 |

[95]:
```
concrete_labels.head()
```

[95]:
```
362    61.990787
233    53.903234
289     7.315340
737    17.540269
139    63.397318
```

```
Name: strength, dtype: float64
```

### 1.5.2 Data cleaning

**Look at the rows with NaN value**

[96]:
```python
null_rows_idx = concrete.isnull().any(axis=1)
concrete.loc[null_rows_idx].head()
```

[96]:
```
Empty DataFrame
Columns: [cement, slag, ash, water, superplastic, coarseagg, fineagg, age]
Index: []
```

[97]:
```python
from sklearn.preprocessing import StandardScaler
std_scaler = StandardScaler()
```

## 1.6 Feature Scaling and Transformation

### 1.6.1 Build Pipeline

[98]:
```python
from sklearn.pipeline import make_pipeline
from sklearn.compose import ColumnTransformer
from sklearn.preprocessing import FunctionTransformer
from sklearn.compose import make_column_selector
from sklearn.impute import SimpleImputer

def ratio_pipeline():
    return make_pipeline(
        SimpleImputer(strategy="median"),
        FunctionTransformer(column_ratio, feature_names_out=ratio_name),
        StandardScaler())

def column_ratio(X):
    return X[:, [0]] / X[:, [1]]

def ratio_name(function_transformer, feature_names_in):
    return ["ratio"] # feature names out

def log_pipeline():
    return make_pipeline(
        SimpleImputer(strategy="median"),
        FunctionTransformer(np.log1p, feature_names_out="one-to-one"),
        StandardScaler())

def cat_pipeline():
    return make_pipeline(
        SimpleImputer(strategy="most_frequent"),
        OneHotEncoder(handle_unknown="ignore"))
```

```python
def default_num_pipeline():
    return make_pipeline(
        SimpleImputer(strategy="median"),
        StandardScaler())

preprocessing = ColumnTransformer([
("cement_water", ratio_pipeline(),
 ["cement", "water"]),
 ("age_water", ratio_pipeline(),
 ["age", "water"]),
 ("log", log_pipeline(),
 ["cement", "water", "superplastic", "fineagg"]),
],remainder=default_num_pipeline())
# remaining col: housing_median_age

housing_prepared = preprocessing.fit_transform(concrete)
housing_prepared.shape
```

[98]: (875, 9)

## 1.7 Select and Train a Model

housing.head()

[99]:
```python
concrete.head()
```

[99]:

| | cement | slag | ash | water | superplastic | coarseagg | fineagg | age |
|---|---|---|---|---|---|---|---|---|
| 362 | 218.23 | 54.64 | 123.78 | 140.75 | 11.91 | 1075.7 | 792.67 | 56 |
| 233 | 213.72 | 98.05 | 24.51 | 181.71 | 6.86 | 1065.8 | 785.38 | 100 |
| 289 | 182.04 | 45.21 | 121.97 | 170.21 | 8.19 | 1059.4 | 780.65 | 3 |
| 737 | 238.00 | 0.00 | 0.00 | 186.00 | 0.00 | 1119.0 | 789.00 | 28 |
| 139 | 374.00 | 189.20 | 0.00 | 170.10 | 10.10 | 926.1 | 756.70 | 56 |

[100]:
```python
from sklearn.linear_model import LinearRegression
from sklearn.metrics import root_mean_squared_error
from sklearn.metrics import mean_squared_error
lin_reg = make_pipeline(preprocessing, LinearRegression())
lin_reg.fit(concrete, concrete_labels)
concrete_predictions = lin_reg.predict(concrete)
lin_rmse = mean_squared_error(concrete_labels,␣
 ↪concrete_predictions,squared=False)

lin_rmse
```

```
c:\Users\dania\AppData\Local\Programs\Python\Python312\Lib\site-
packages\sklearn\metrics\_regression.py:483: FutureWarning: 'squared' is
```

deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function'root_mean_squared_error'.
  warnings.warn(

[100]: 9.901323990721124

### 1.7.1 Example 2 - Decision Tree Model

[101]:
```
from sklearn.tree import DecisionTreeRegressor
tree_reg = make_pipeline(preprocessing, DecisionTreeRegressor(random_state=42))
tree_reg.fit(concrete, concrete_labels)
concrete_predictions = tree_reg.predict(concrete)
tree_rmse = mean_squared_error(concrete_labels,␣
↪concrete_predictions,squared=False)

tree_rmse
```

```
c:\Users\dania\AppData\Local\Programs\Python\Python312\Lib\site-
packages\sklearn\metrics\_regression.py:483: FutureWarning: 'squared' is
deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean
squared error, use the function'root_mean_squared_error'.
  warnings.warn(
```

[101]: 0.920606779688016

### 1.7.2 Example 3 - Random Forest Regressor

[102]:
```
from sklearn.ensemble import RandomForestRegressor
forest_reg = make_pipeline(preprocessing,
                           RandomForestRegressor(random_state=42))
forest_reg.fit(concrete, concrete_labels)
housing_predictions = forest_reg.predict(concrete)
forest_rmse = mean_squared_error(concrete_labels,␣
↪housing_predictions,squared=False)

forest_rmse
```

```
c:\Users\dania\AppData\Local\Programs\Python\Python312\Lib\site-
packages\sklearn\metrics\_regression.py:483: FutureWarning: 'squared' is
deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean
squared error, use the function'root_mean_squared_error'.
  warnings.warn(
```

[102]: 2.0314085819778542

### 1.7.3 Cross Validation

[103]:
```
from sklearn.model_selection import cross_val_score
```

### 1.7.4 Cross Validate Example 1

[104]:
```
lin_rmses = -cross_val_score(lin_reg, concrete, concrete_labels,
scoring="neg_root_mean_squared_error", cv=10)
print("Cross-validation RMSEs (Kfold):", lin_rmses)
print("Mean:", lin_rmses.mean())
```

```
Cross-validation RMSEs (Kfold): [10.98119705  9.43062432  9.9105226   9.4939674
9.48025498 10.54156651
 10.19910391  8.86058674  9.89249137 11.32818057]
Mean: 10.011849544101992
```

### 1.7.5 Cross Validate Example 2

[105]:
```
tree_rmses = -cross_val_score(tree_reg, concrete, concrete_labels,
scoring="neg_root_mean_squared_error", cv=10)
print("Cross-validation RMSEs (Kfold):", tree_rmses.mean())
print("Mean:", tree_rmses.mean())
```

```
Cross-validation RMSEs (Kfold): 6.638941906141537
Mean: 6.638941906141537
```

### 1.7.6 Cross Validate Example 3

[106]:
```
forest_rmses = -cross_val_score(forest_reg, concrete, concrete_labels,
scoring="neg_root_mean_squared_error", cv=10)
print("Cross-validation RMSEs (Kfold):", forest_rmses.mean())
```

```
Cross-validation RMSEs (Kfold): 5.1655086457549935
```

## 1.8 Model Fine-tuning

[107]:
```
from sklearn.pipeline import Pipeline
full_pipeline = Pipeline([
    ("preprocessing", preprocessing),
    ("random_forest", RandomForestRegressor(random_state=42)),
])
```

### 1.8.1 Option 1 (Grid Search)

[108]:
```
from sklearn.model_selection import GridSearchCV

param_grid = [
```

```
{'random_forest__max_features': [2,4,6,8,10,12,14,16]}
]

grid_search = GridSearchCV(full_pipeline, param_grid, cv=3,
scoring='neg_root_mean_squared_error')

grid_search.fit(concrete, concrete_labels)
final_model = grid_search.best_estimator_

cv_res = pd.DataFrame(grid_search.cv_results_)
cv_res.sort_values(by="mean_test_score", ascending=False, inplace=True)
best_hyperparameters_grid = grid_search.best_params_
best_max_features = best_hyperparameters_grid['random_forest__max_features']


feature_importances = final_model["random_forest"].feature_importances_
feature_importances.round(2)

sorted(zip(feature_importances,
           final_model["preprocessing"].get_feature_names_out()),
       reverse=True)
```

[108]:
```
[(0.43488673889891305, 'age_water__ratio'),
 (0.21207136034410806, 'cement_water__ratio'),
 (0.10252755661497995, 'log__cement'),
 (0.05226666720648145, 'remainder__slag'),
 (0.04860179079548339, 'log__water'),
 (0.04845608420794533, 'log__superplastic'),
 (0.045310382607353185, 'log__fineagg'),
 (0.03498547167428484, 'remainder__coarseagg'),
 (0.020893947650450776, 'remainder__ash')]
```

### 1.8.2 Option 2 (Randomised Search)

[109]:
```
from sklearn.model_selection import RandomizedSearchCV
from scipy.stats import randint

param_distribs = {'random_forest__max_features': randint(low=2, high=20)}

rnd_search = RandomizedSearchCV(
full_pipeline, param_distributions=param_distribs, n_iter=10, cv=3,
scoring='neg_root_mean_squared_error', random_state=42)

rnd_search.fit(concrete, concrete_labels)
final_model2 = rnd_search.best_estimator_

cv_res2 = pd.DataFrame(rnd_search.cv_results_)
```

```python
cv_res2.sort_values(by="mean_test_score", ascending=False, inplace=True)
best_hyperparameters_rnd = rnd_search.best_params_
best_max_features = best_hyperparameters_rnd['random_forest__max_features']


feature_importances = final_model2["random_forest"].feature_importances_
feature_importances.round(2)

sorted(zip(feature_importances,
           final_model2["preprocessing"].get_feature_names_out()),
       reverse=True)
```

[109]:
```
[(0.449435017971098, 'age_water__ratio'),
 (0.22057918150618364, 'cement_water__ratio'),
 (0.1072048323684825, 'log__cement'),
 (0.05866177408859303, 'remainder__slag'),
 (0.04114782424311172, 'log__water'),
 (0.039732646977352, 'log__superplastic'),
 (0.03876660183062856, 'log__fineagg'),
 (0.027862939226582933, 'remainder__coarseagg'),
 (0.016609181787967765, 'remainder__ash')]
```

### 1.8.3 Evaluate Model on Test Set

[115]:
```python
print("Random Forest Grid")
X_test = strat_test_set.drop("strength", axis=1)
y_test = strat_test_set["strength"].copy()
final_predictions = final_model.predict(X_test)
final_rmse = mean_squared_error(y_test, final_predictions, squared=False)
print(final_rmse)
```

```
Random Forest Grid
3.7884011156215167
```

```
c:\Users\dania\AppData\Local\Programs\Python\Python312\Lib\site-
packages\sklearn\metrics\_regression.py:483: FutureWarning: 'squared' is
deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean
squared error, use the function'root_mean_squared_error'.
  warnings.warn(
```

[111]:
```python
print("Random Forest Randomized")
X_test = strat_test_set.drop("strength", axis=1)
y_test = strat_test_set["strength"].copy()
final_predictions = final_model2.predict(X_test)
final_rmse = mean_squared_error(y_test, final_predictions, squared=False)
print(final_rmse)
```

```
Random Forest Randomized
```

```
3.974520424808947
```

```
c:\Users\dania\AppData\Local\Programs\Python\Python312\Lib\site-
packages\sklearn\metrics\_regression.py:483: FutureWarning: 'squared' is
deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean
squared error, use the function'root_mean_squared_error'.
  warnings.warn(
```

### 1.8.4 Random Forest Grid will be used as final model prediction

[116]:
```
from scipy import stats
confidence = 0.95
squared_errors = (final_predictions - y_test) ** 2
np.sqrt(stats.t.interval(confidence, len(squared_errors) - 1,
                         loc=squared_errors.mean(),
                         scale=stats.sem(squared_errors)))
```

[116]:
```
array([3.12703445, 4.35035879])
```