Questions

1. Is there a relationship between the predictors (age and ingredients) and the response variable (compressive strength)?

Given there is a relationship:

2. How strong is it?
3. Which predictors contribute to compressive strength?
4. How large is the effect of each predictor on compressive strength?
5. How accurately can I predict compressive strength?
6. Is the relationship linear?
7. Is there synergy/interaction among the predictors?

1. Import packages and Data

In [1]:
```
#import standard packages
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns; sns.set()

#supress warnings
import warnings
warnings.filterwarnings("ignore")
```

In [2]:
```
#import data
concrete_data = pd.read_csv('../input/yeh-concret-data/Concrete_Data_Yeh.csv')
```

2. Initial EDA and Distributions

In [3]:
```
#look at formatting of entries
concrete_data.head()
```

Out[3]:

	cement	slag	flyash	water	superplasticizer	coarseaggregate	fineaggregate	age
0	540.0	0.0	0.0	162.0	2.5	1040.0	676.0	28
1	540.0	0.0	0.0	162.0	2.5	1055.0	676.0	28
2	332.5	142.5	0.0	228.0	0.0	932.0	594.0	270
3	332.5	142.5	0.0	228.0	0.0	932.0	594.0	365
4	198.6	132.4	0.0	192.0	0.0	978.4	825.5	360

In [4]:
```
#look at null count and dtype
```

```
concrete_data.info()
```

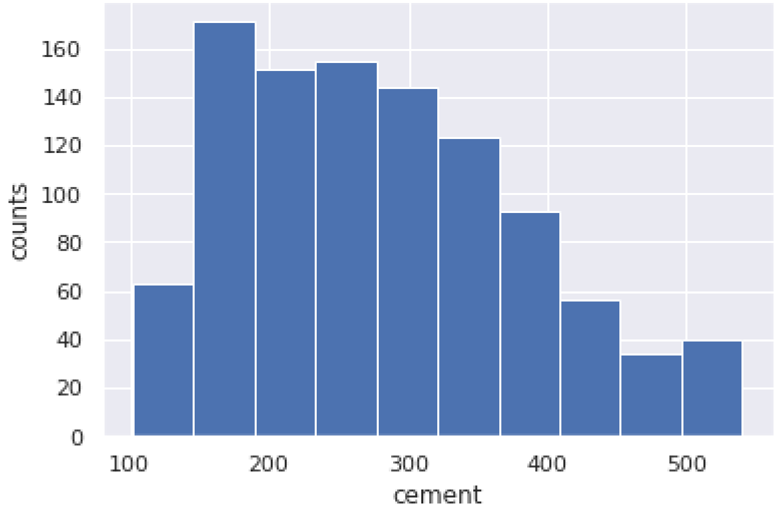
```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1030 entries, 0 to 1029
Data columns (total 9 columns):
 #   Column            Non-Null Count  Dtype  
---  ------            --------------  -----  
 0   cement            1030 non-null   float64
 1   slag              1030 non-null   float64
 2   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
```

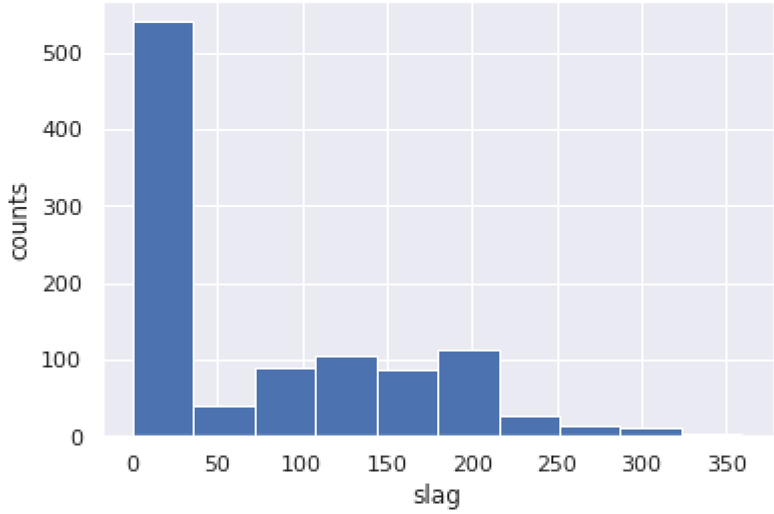
In [5]:
```
#look at distribution of data
concrete_data.describe()
```

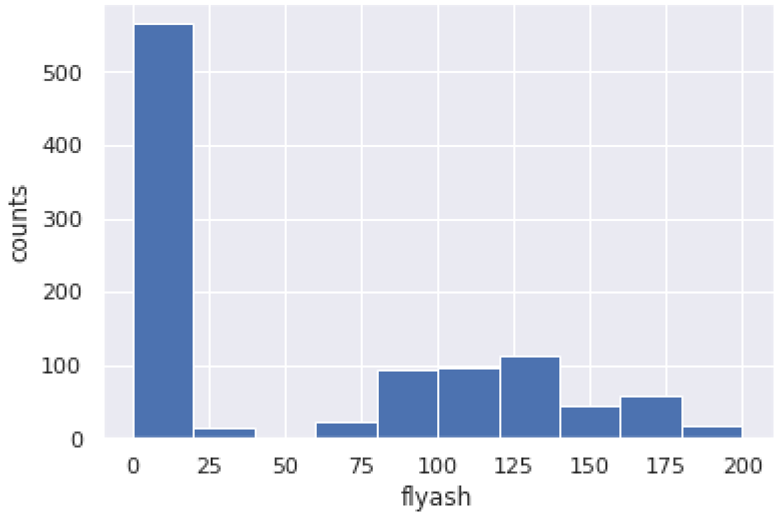
Out[5]:

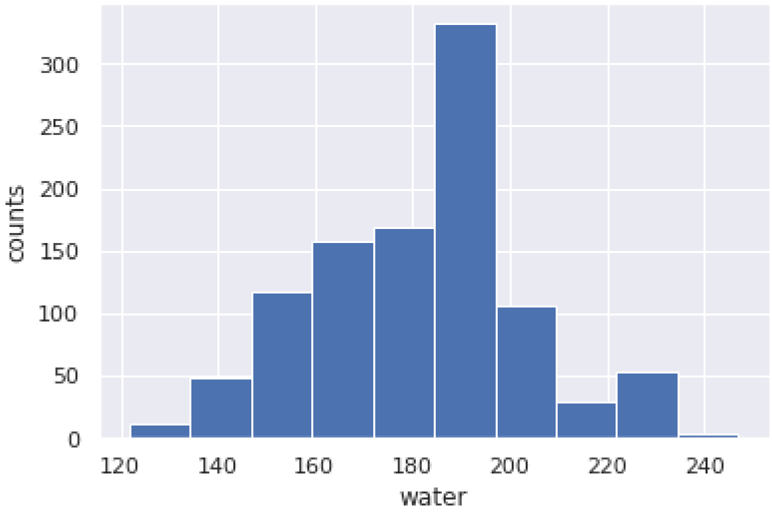
	cement	slag	flyash	water	superplasticizer	coarseaggr
count	1030.000000	1030.000000	1030.000000	1030.000000	1030.000000	1030.0(
mean	281.167864	73.895825	54.188350	181.567282	6.204660	972.9
std	104.506364	86.279342	63.997004	21.354219	5.973841	77.7!
min	102.000000	0.000000	0.000000	121.800000	0.000000	801.0(
25%	192.375000	0.000000	0.000000	164.900000	0.000000	932.0(
50%	272.900000	22.000000	0.000000	185.000000	6.400000	968.0(
75%	350.000000	142.950000	118.300000	192.000000	10.200000	1029.4(
max	540.000000	359.400000	200.100000	247.000000	32.200000	1145.0(

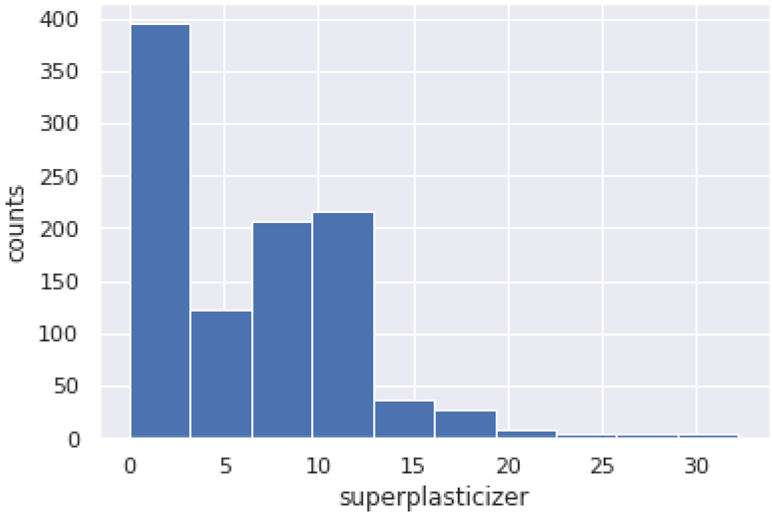
In [6]:
```
#look at data distribution
for i in concrete_data.columns:
    plt.hist(concrete_data[i])
    plt.xticks()
    plt.xlabel(i)
    plt.ylabel('counts')
    plt.show()
```

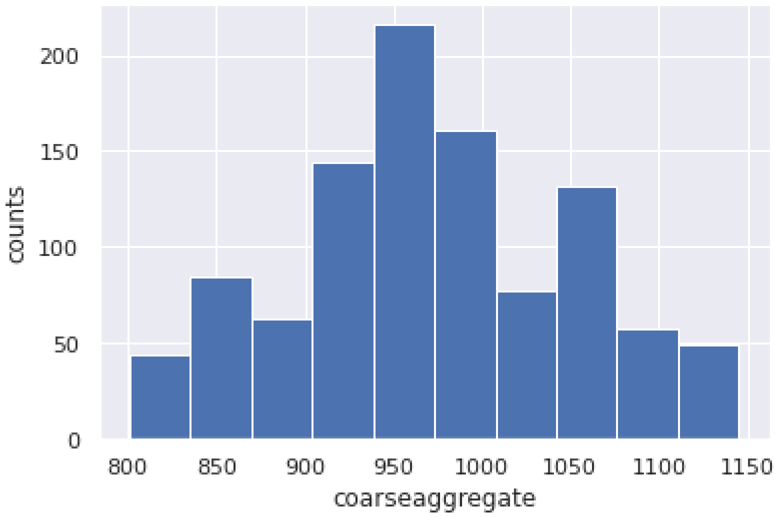

counts
0
20
40
60
80
100
120
140
160
100
200
300
400
500
cement

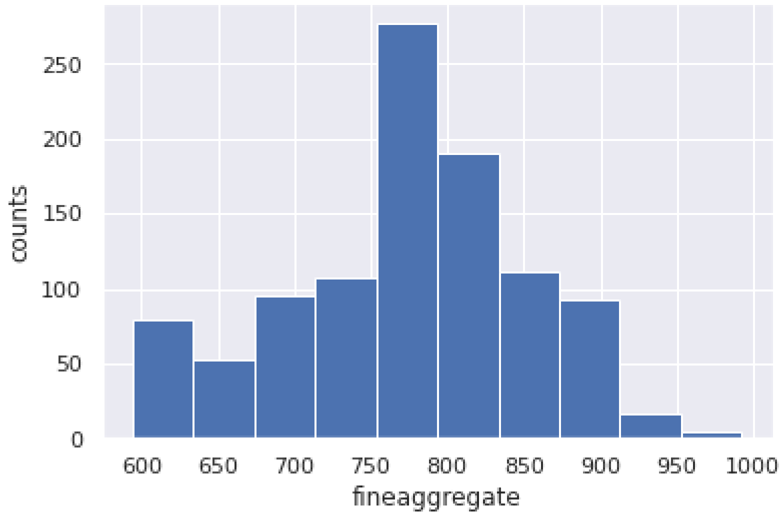

counts
0
100
200
300
400
500
0
50
100
150
200
250
300
350
slag

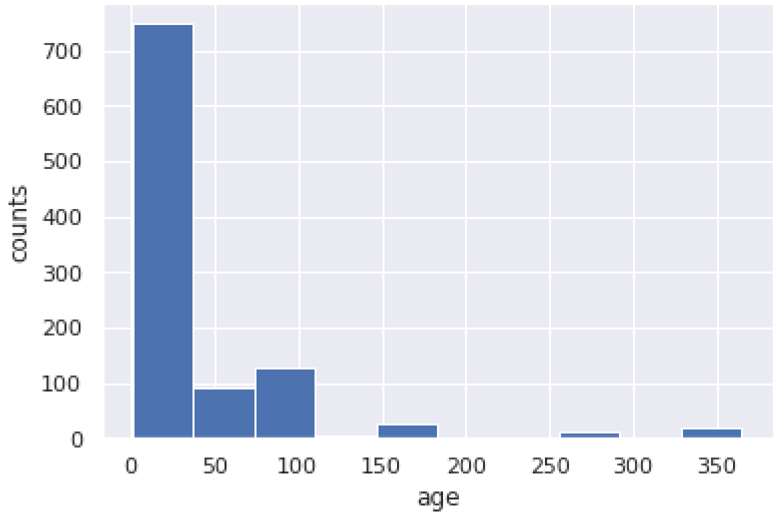

counts
0
100
200
300
400
500
0
25
50
75
100
125
150
175
200
flyash

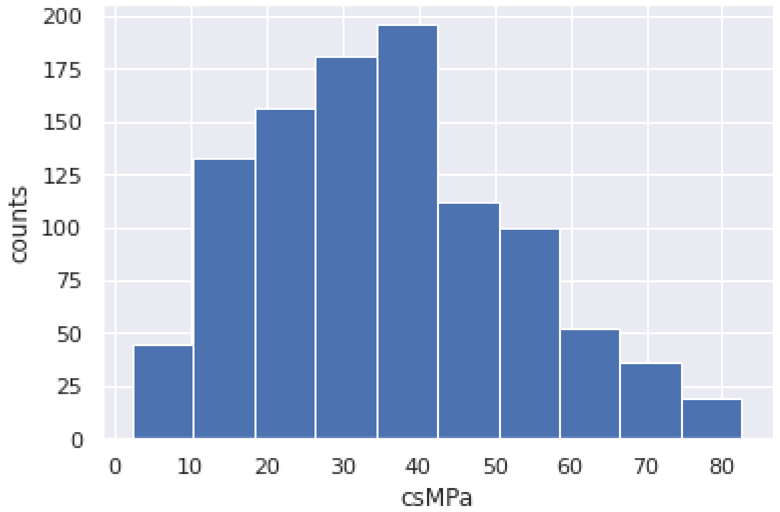

counts
0
50
100
150
200
250
300
120
140
160
180
200
220
240
water


counts
0
50
100
150
200
250
300
350
400
0
5
10
15
20
25
30
superplasticizer

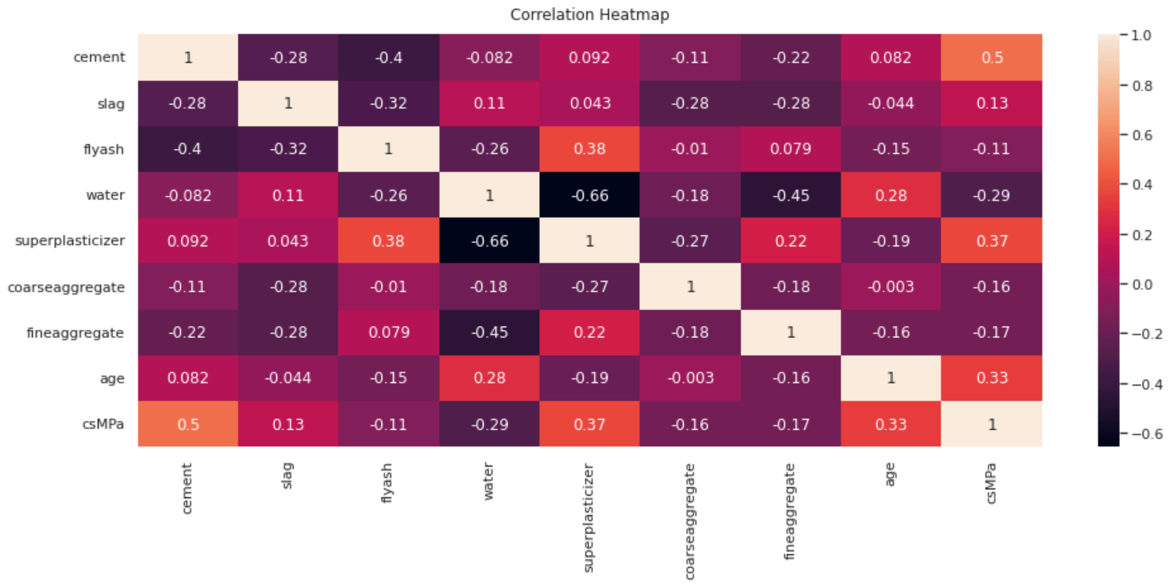

counts
0
50
100
150
200
800
850
900
950
1000
1050
1100
1150
coarseaggregate





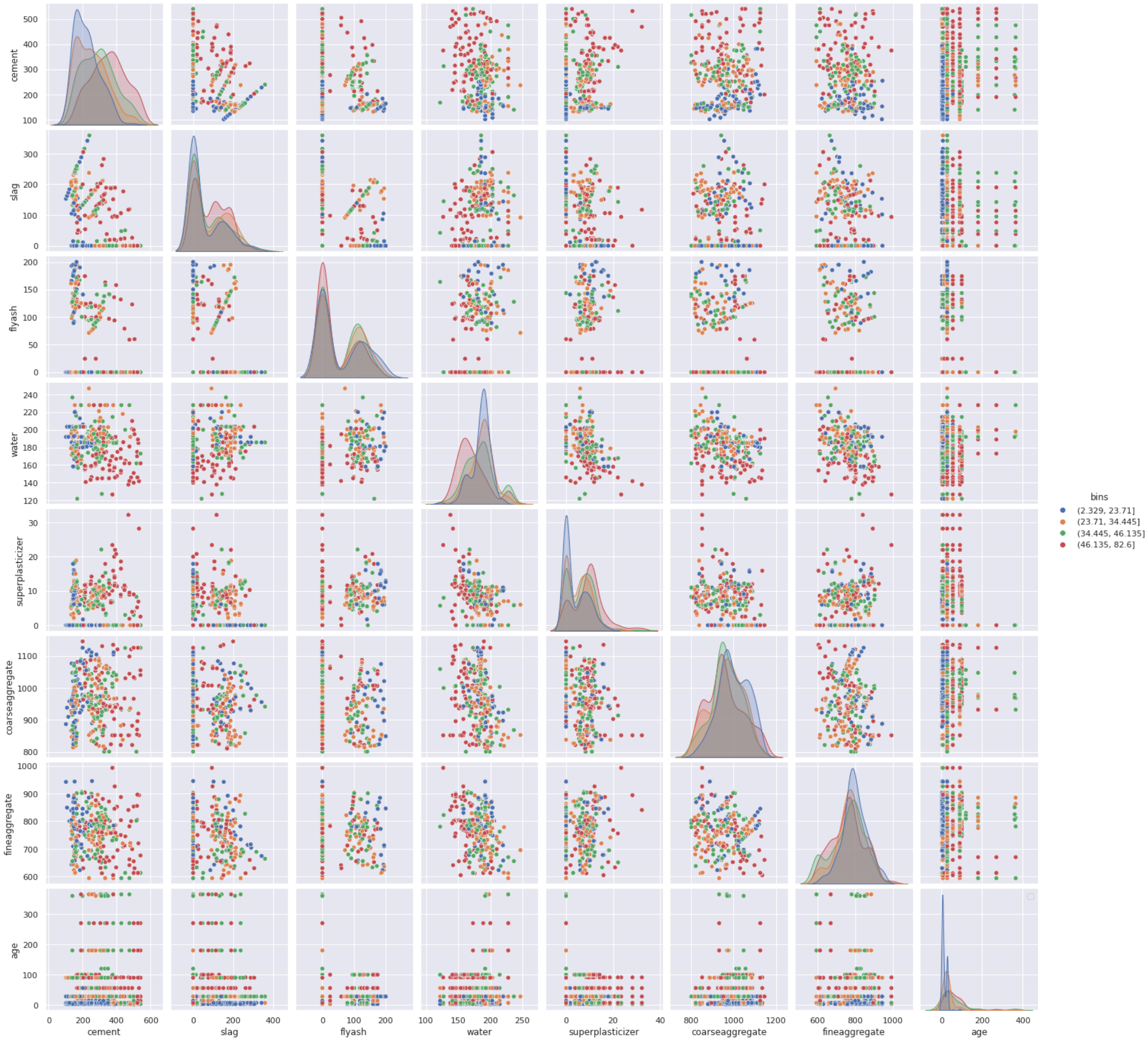


In [7]:
```
#heat map using Pearson's coefficient
plt.figure(figsize=(16, 6))
sns.heatmap(concrete_data.corr(), annot=True)
plt.title('Correlation Heatmap', fontdict={'fontsize':12}, pad=12);
```

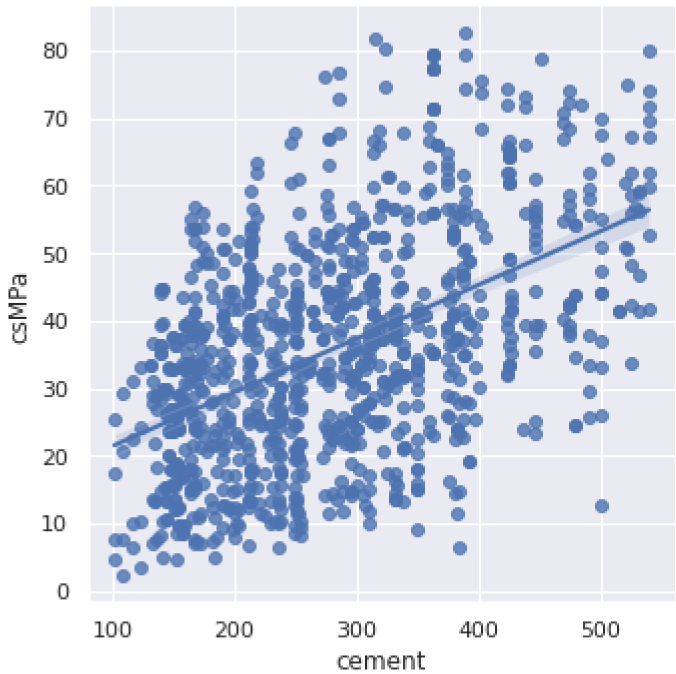


In [8]:
```
#create bins from compressive strength
bins = pd.qcut(concrete_data['csMPa'], q=4)

#add bins to concrete df
concrete_data['bins']=bins
```

In [9]:
```
#look at how target is distributed among variables
sns.pairplot(concrete_data.loc[:, (concrete_data.columns != 'csMPa')], hue='bins
plt.legend()
plt.show()
```



In [10]:
```
#plot strongest linear correlation
sns.lmplot(x='cement', y='csMPa',data=concrete_data)
plt.show()
```



In [11]:
```
#drop bins from concrete data
concrete_data = concrete_data.drop('bins', axis=1)
```

In [12]:
```
#copy of variables and target
X = concrete_data.copy()
y = X.pop('csMPa')
```

3. Mutual Information

In [13]:
```
#make a copy of features matrix for mutual information analysis
X_mi = X.copy()

#label encoding for categorical variables
for colname in X_mi.select_dtypes("object"):
    X_mi[colname], _ = X_mi[colname].factorize()

#all discrete features have int dtypes
discrete_features = X_mi.dtypes == object
```

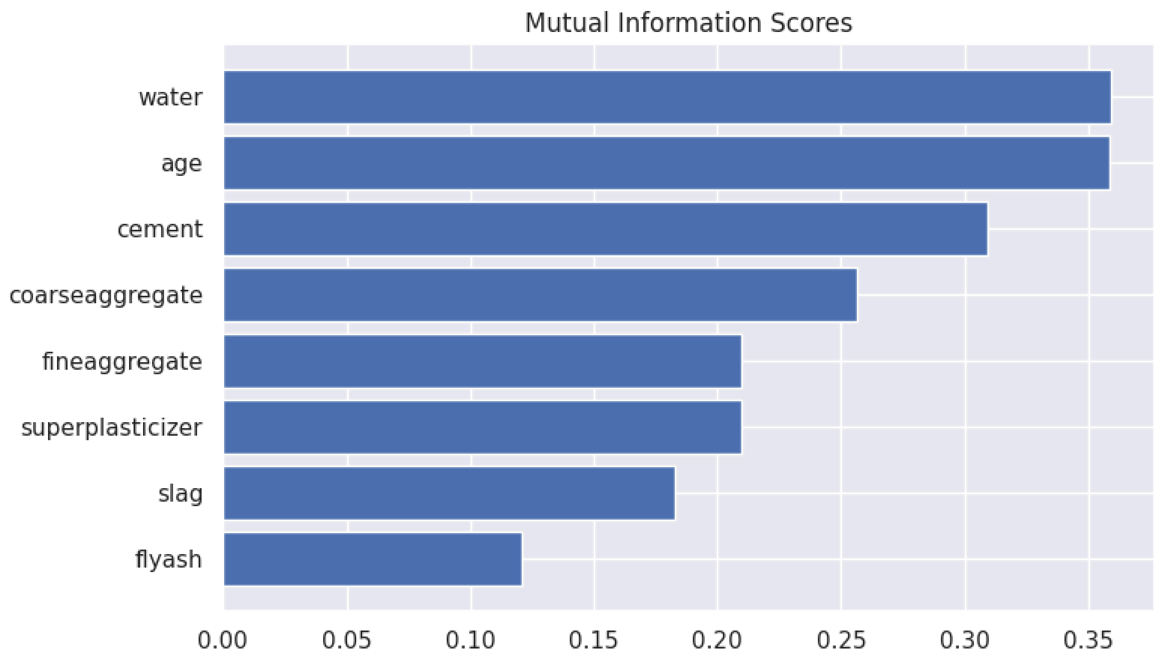
In [14]:
```
#some continuous variables also have int dtypes
discrete_features[X_mi.columns] = False
```

In [15]:
```
#use regression since the target variable is continuous
from sklearn.feature_selection import mutual_info_regression

#define a function to produce mutual information scores
def make_mi_scores(X_mi, y, discrete_features):
    mi_scores = mutual_info_regression(X_mi, y, discrete_features=discrete_featu
    mi_scores = pd.Series(mi_scores, name="MI Scores", index=X_mi.columns)
    mi_scores = mi_scores.sort_values(ascending=False)
    return mi_scores

#compute mutual information scores
mi_scores = make_mi_scores(X_mi, y, discrete_features)
mi_scores
```

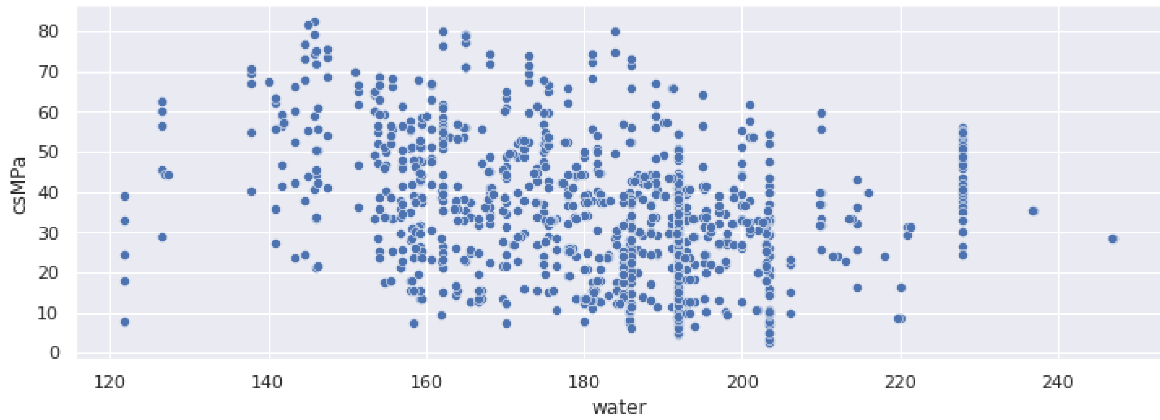
Out[15]:
```
water               0.359076
age                 0.358395
cement              0.309544
coarseaggregate     0.256413
fineaggregate       0.209647
superplasticizer    0.209488
slag                0.183057
flyash              0.120885
Name: MI Scores, dtype: float64
```

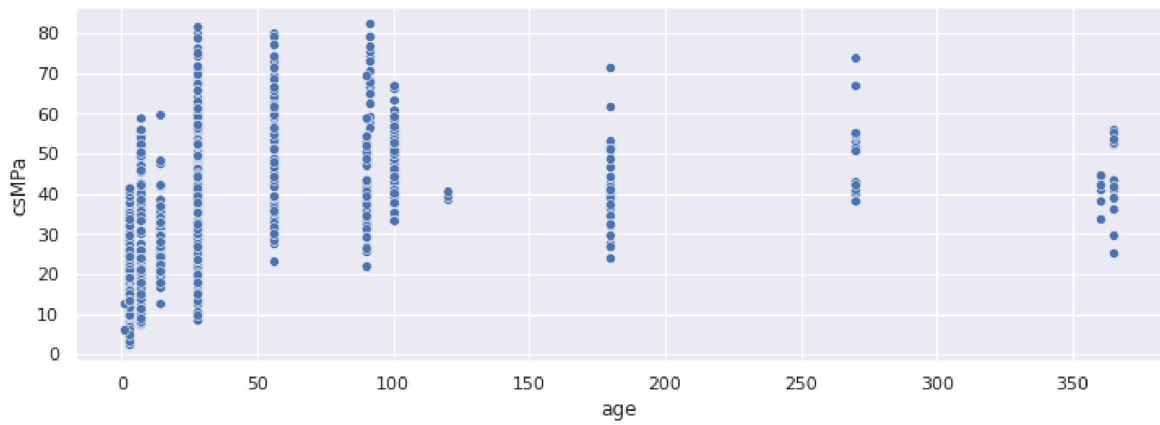
In [16]:
```
#define a function to plot mutual information scores
def plot_mi_scores(scores):
    scores = scores.sort_values(ascending=True)
    width = np.arange(len(scores))
    ticks = list(scores.index)
    plt.barh(width, scores)
    plt.yticks(width, ticks)
    plt.title("Mutual Information Scores")

#plot the scores
```

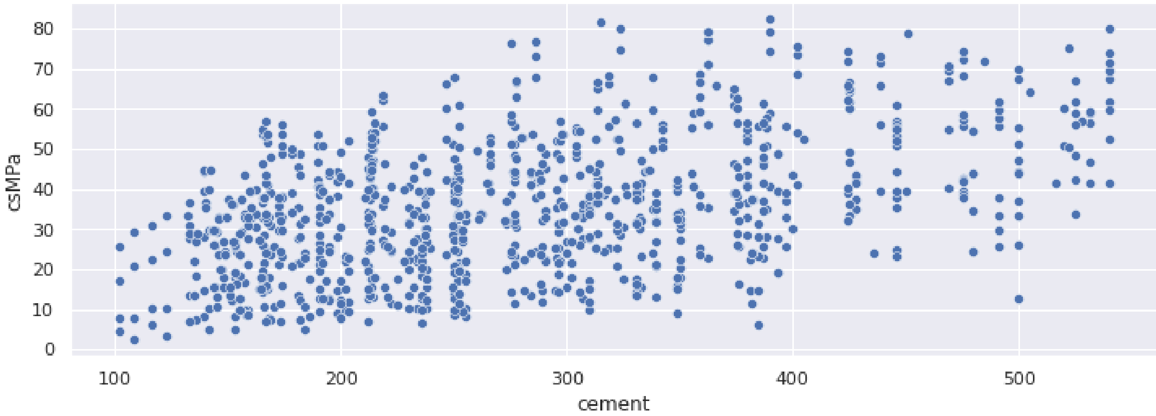
```
plt.figure(dpi=100, figsize=(8, 5))
plot_mi_scores(mi_scores)
```



In [17]:
```
#plot top MI score predictors against target
for i in ['water', 'age', 'cement']:
    fig, ax = plt.subplots(figsize=(12,4))
    sns.scatterplot(x=X_mi[i], y=y, ax=ax)
    plt.show()
```



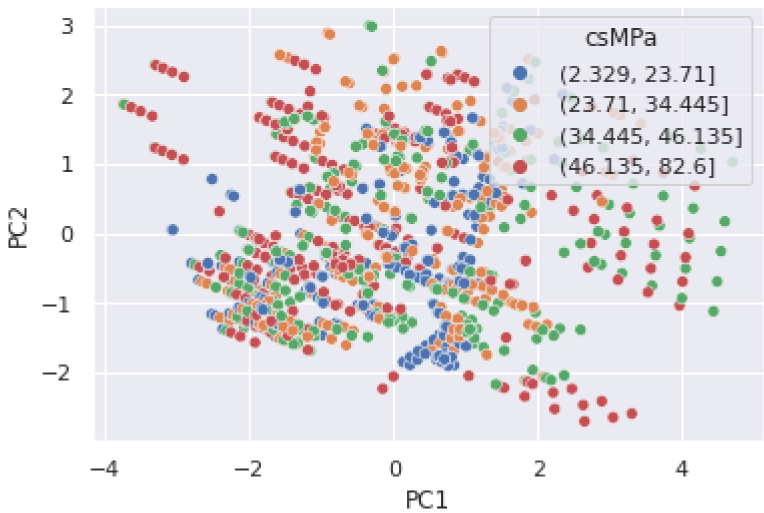




4. Principal Component Analysis

In [18]:
```
#copy features matrix for principal component analysis
X_for_PCA = X.copy()

#standardize
X_for_PCA_scaled = (X_for_PCA - X_for_PCA.mean(axis=0)) / X_for_PCA.std(axis=0)

from sklearn.decomposition import PCA

#create principal components
pca = PCA(len(X.columns))
X_pca = pca.fit_transform(X_for_PCA_scaled)

#convert to dataframe
component_names = [f"PC{i+1}" for i in range(X_pca.shape[1])]
X_pca = pd.DataFrame(X_pca, columns=component_names)
```

In [19]:
```
#plot data using principal components
sns.scatterplot(x=X_pca.loc[:,'PC1'],y=X_pca.loc[:,'PC2'], hue=bins)
plt.show()
```



In [20]:
```
#determine loadings
loadings = pd.DataFrame(
    pca.components_.T,  # transpose the matrix of loadings
    columns=component_names,  # so the columns are the principal components
    index=X.columns,  # and the rows are the original features
```

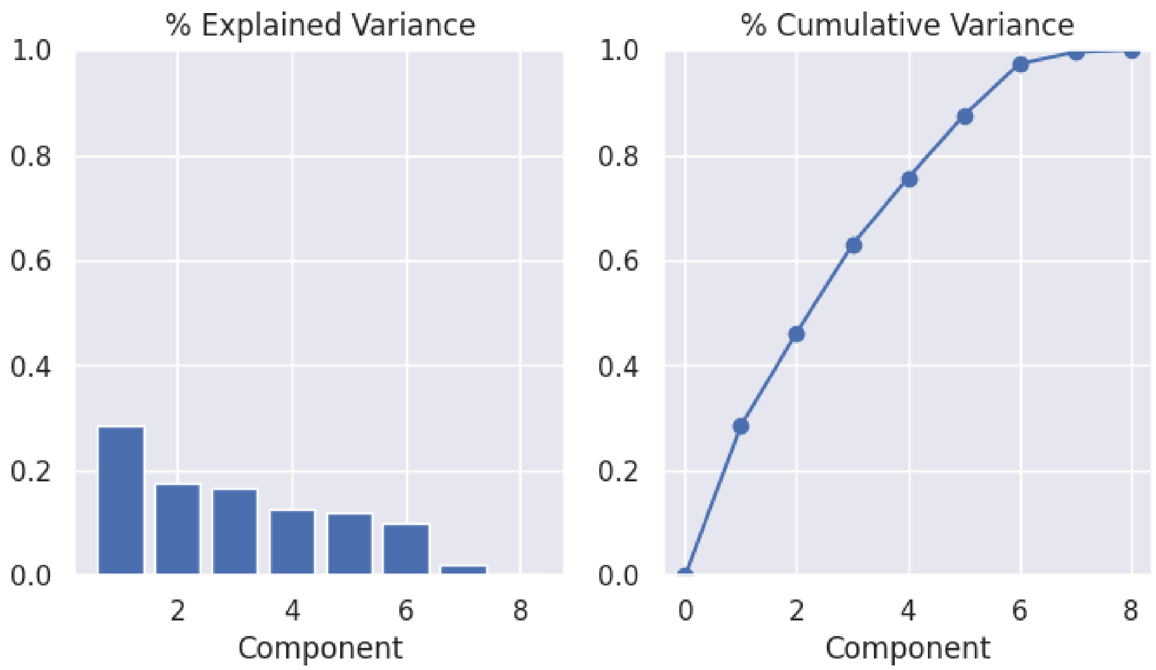
```
)
loadings
```

Out[20]:

	PC1	PC2	PC3	PC4	PC5	PC6	
cement	0.098401	-0.113737	0.814202	-0.054297	0.148206	-0.203142	0.221
slag	0.177262	0.686053	-0.171794	-0.362699	-0.020932	0.304882	0.228
flyash	-0.394662	-0.142948	-0.408221	0.226751	0.549631	-0.183267	0.352
water	0.547004	0.053256	-0.213190	0.296060	0.070222	-0.365970	-0.524
superplasticizer	-0.505945	0.282930	0.234597	-0.037274	0.354618	0.193294	-0.664
coarseaggregate	0.037928	-0.629943	-0.174088	-0.545805	-0.033083	0.314559	-0.226
fineaggregate	-0.401926	-0.019391	-0.004569	0.385282	-0.701237	0.092466	-0.039
age	0.291479	-0.125981	0.100521	0.527919	0.228010	0.743908	0.069

In [21]:

```
#determine % explained variance and use % cumulative variance for elbow method t

def plot_variance(pca, width=8, dpi=100):
    # Create figure
    fig, axs = plt.subplots(1, 2)
    n = pca.n_components_
    grid = np.arange(1, n + 1)
    # Explained variance
    evr = pca.explained_variance_ratio_
    axs[0].bar(grid, evr)
    axs[0].set(
        xlabel="Component", title="% Explained Variance", ylim=(0.0, 1.0)
    )
    # Cumulative Variance
    cv = np.cumsum(evr)
    axs[1].plot(np.r_[0, grid], np.r_[0, cv], "o-")
    axs[1].set(
        xlabel="Component", title="% Cumulative Variance", ylim=(0.0, 1.0)
    )
    # Set up figure
    fig.set(figwidth=8, dpi=100)
    return axs

plot_variance(pca);
```



5. OLS Regression Analysis

In [22]:

```
#generate OLS regression results for all features
import statsmodels.api as sm

X_sm = sm.add_constant(X)
model = sm.OLS(y,X_sm)
print(model.fit().summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                  csMPa   R-squared:                       0.616
Model:                            OLS   Adj. R-squared:                  0.613
Method:                 Least Squares   F-statistic:                     204.3
Date:                Fri, 15 Oct 2021   Prob (F-statistic):          6.29e-206
Time:                        16:43:15   Log-Likelihood:                -3869.0
No. Observations:                1030   AIC:                             7756.
Df Residuals:                    1021   BIC:                             7800.
Df Model:                           8
Covariance Type:            nonrobust
================================================================================
===
                       coef    std err          t      P>|t|      [0.025      0.9
75]
--------------------------------------------------------------------------------
---
const              -23.3312     26.586     -0.878      0.380     -75.500      28.
837
cement               0.1198      0.008     14.113      0.000       0.103       0.
136
slag                 0.1039      0.010     10.247      0.000       0.084       0.
124
flyash               0.0879      0.013      6.988      0.000       0.063       0.
113
water               -0.1499      0.040     -3.731      0.000      -0.229      -0.
071
superplasticizer     0.2922      0.093      3.128      0.002       0.109       0.
476
coarseaggregate      0.0181      0.009      1.926      0.054      -0.000       0.
037
fineaggregate        0.0202      0.011      1.887      0.059      -0.001       0.
041
age                  0.1142      0.005     21.046      0.000       0.104       0.
125
==============================================================================
Omnibus:                        5.378   Durbin-Watson:                   1.282
Prob(Omnibus):                  0.068   Jarque-Bera (JB):                5.304
Skew:                          -0.174   Prob(JB):                       0.0705
Kurtosis:                       3.045   Cond. No.                     1.06e+05
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
[2] The condition number is large, 1.06e+05. This might indicate that there are
strong multicollinearity or other numerical problems.
```

In [23]:

```python
from statsmodels.stats.outliers_influence import variance_inflation_factor

#initialize VIF dataframe
vif_data = pd.DataFrame()
vif_data["feature"] = X.columns

#calculate VIF for each feature
vif_data["VIF"] = [variance_inflation_factor(X.values, i)
                          for i in range(len(X.columns))]

print(vif_data)
```

	feature	VIF
0	cement	15.456717
1	slag	3.329127
2	flyash	4.147833
3	water	82.157569
4	superplasticizer	5.471094
5	coarseaggregate	84.955779
6	fineaggregate	72.790995
7	age	1.699459

In [24]:

```
#print OLS summary for each feature
for i in X.columns:
    X_sm = sm.add_constant(X[i])
    model = sm.OLS(y,X_sm)
    print(model.fit().summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                  csMPa   R-squared:                       0.248
Model:                            OLS   Adj. R-squared:                  0.247
Method:                 Least Squares   F-statistic:                     338.7
Date:                Fri, 15 Oct 2021   Prob (F-statistic):           1.32e-65
Time:                        16:43:15   Log-Likelihood:                -4214.6
No. Observations:                1030   AIC:                             8433.
Df Residuals:                    1028   BIC:                             8443.
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         13.4425      1.297     10.365      0.000      10.898      15.987
cement         0.0796      0.004     18.404      0.000       0.071       0.088
==============================================================================
Omnibus:                       19.696   Durbin-Watson:                   1.012
Prob(Omnibus):                  0.000   Jarque-Bera (JB):               17.893
Skew:                           0.271   Prob(JB):                     0.000130
Kurtosis:                       2.649   Cond. No.                         861.
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
                            OLS Regression Results
==============================================================================
Dep. Variable:                  csMPa   R-squared:                       0.018
Model:                            OLS   Adj. R-squared:                  0.017
Method:                 Least Squares   F-statistic:                     19.03
Date:                Fri, 15 Oct 2021   Prob (F-statistic):           1.41e-05
Time:                        16:43:15   Log-Likelihood:                -4351.8
No. Observations:                1030   AIC:                             8708.
Df Residuals:                    1028   BIC:                             8717.
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         33.8888      0.680     49.868      0.000      32.555      35.222
slag           0.0261      0.006      4.363      0.000       0.014       0.038
==============================================================================
Omnibus:                       30.576   Durbin-Watson:                   0.860
Prob(Omnibus):                  0.000   Jarque-Bera (JB):               28.559
Skew:                           0.359   Prob(JB):                     6.29e-07
Kurtosis:                       2.614   Cond. No.                         150.
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
                            OLS Regression Results
==============================================================================
Dep. Variable:                  csMPa   R-squared:                       0.011
Model:                            OLS   Adj. R-squared:                  0.010
Method:                 Least Squares   F-statistic:                     11.63
Date:                Fri, 15 Oct 2021   Prob (F-statistic):           0.000675
Time:                        16:43:15   Log-Likelihood:                -4355.4
No. Observations:                1030   AIC:                             8715.
```

```
Df Residuals:                    1028   BIC:                             8725.
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         37.3139      0.679     54.978      0.000      35.982      38.646
flyash        -0.0276      0.008     -3.410      0.001      -0.043      -0.012
==============================================================================
Omnibus:                       29.013   Durbin-Watson:                   0.848
Prob(Omnibus):                  0.000   Jarque-Bera (JB):               27.218
Skew:                           0.351   Prob(JB):                     1.23e-06
Kurtosis:                       2.625   Cond. No.                         110.
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
                            OLS Regression Results
==============================================================================
Dep. Variable:                  csMPa   R-squared:                       0.084
Model:                            OLS   Adj. R-squared:                  0.083
Method:                 Least Squares   F-statistic:                     94.13
Date:                Fri, 15 Oct 2021   Prob (F-statistic):           2.35e-21
Time:                        16:43:15   Log-Likelihood:                -4316.1
No. Observations:                1030   AIC:                             8636.
Df Residuals:                    1028   BIC:                             8646.
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         76.9583      4.270     18.025      0.000      68.580      85.336
water         -0.2266      0.023     -9.702      0.000      -0.272      -0.181
==============================================================================
Omnibus:                       33.415   Durbin-Watson:                   0.970
Prob(Omnibus):                  0.000   Jarque-Bera (JB):               24.861
Skew:                           0.282   Prob(JB):                     3.99e-06
Kurtosis:                       2.488   Cond. No.                     1.57e+03
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
[2] The condition number is large, 1.57e+03. This might indicate that there are
strong multicollinearity or other numerical problems.
                            OLS Regression Results
==============================================================================
Dep. Variable:                  csMPa   R-squared:                       0.134
Model:                            OLS   Adj. R-squared:                  0.133
Method:                 Least Squares   F-statistic:                     159.1
Date:                Fri, 15 Oct 2021   Prob (F-statistic):           5.13e-34
Time:                        16:43:15   Log-Likelihood:                -4287.1
No. Observations:                1030   AIC:                             8578.
Df Residuals:                    1028   BIC:                             8588.
Df Model:                           1
Covariance Type:            nonrobust
=================================================================================
===
                       coef    std err          t      P>|t|      [0.025      0.9
```

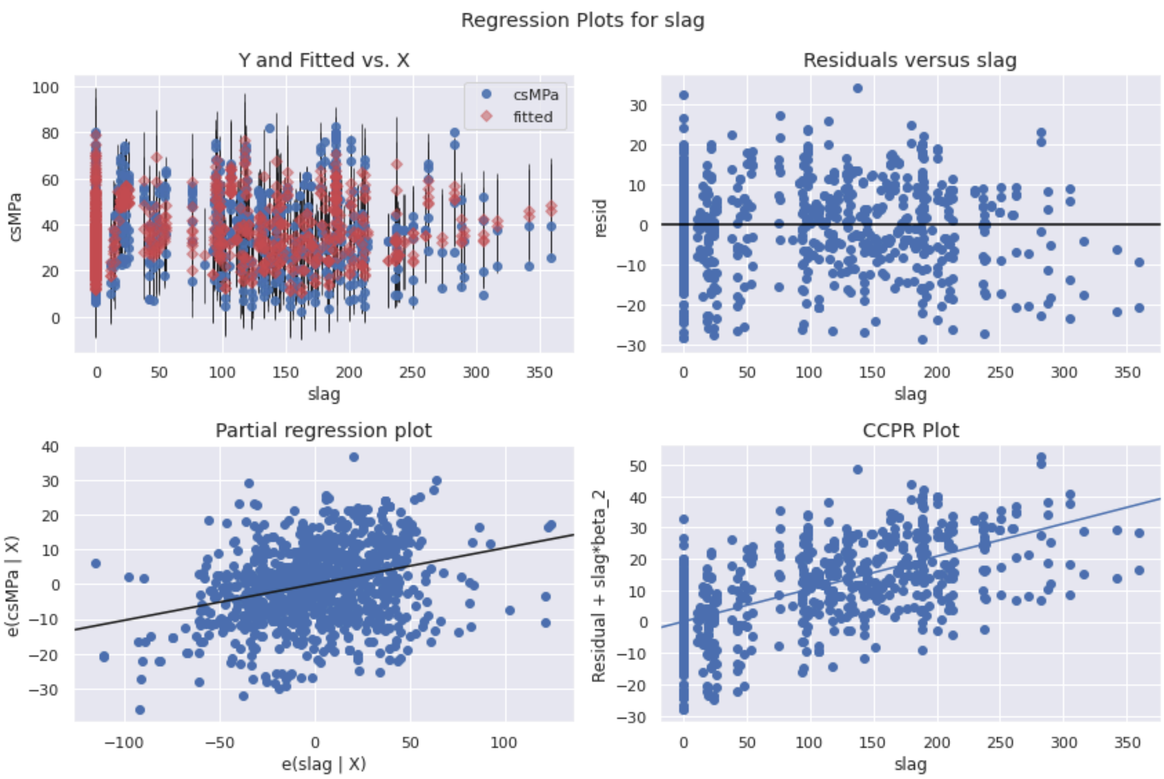
```
75]
------------------------------------------------------------------------------------
---
const               29.4660      0.699     42.159      0.000      28.095      30.
838
superplasticizer     1.0237      0.081     12.613      0.000       0.864       1.
183
==============================================================================
Omnibus:                       24.083   Durbin-Watson:                   1.052
Prob(Omnibus):                  0.000   Jarque-Bera (JB):               24.389
Skew:                           0.353   Prob(JB):                     5.06e-06
Kurtosis:                       2.738   Cond. No.                         12.5
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
                            OLS Regression Results
==============================================================================
Dep. Variable:                  csMPa   R-squared:                       0.027
Model:                            OLS   Adj. R-squared:                  0.026
Method:                 Least Squares   F-statistic:                     28.75
Date:                Fri, 15 Oct 2021   Prob (F-statistic):           1.02e-07
Time:                        16:43:15   Log-Likelihood:                -4347.0
No. Observations:                1030   AIC:                             8698.
Df Residuals:                    1028   BIC:                             8708.
Df Model:                           1
Covariance Type:            nonrobust
==================================================================================
==
                      coef    std err          t      P>|t|      [0.025      0.97
5]
----------------------------------------------------------------------------------
--
const              70.2951      6.451     10.897      0.000      57.637      82.9
53
coarseaggregate    -0.0354      0.007     -5.362      0.000      -0.048      -0.0
22
==============================================================================
Omnibus:                       32.683   Durbin-Watson:                   0.883
Prob(Omnibus):                  0.000   Jarque-Bera (JB):               34.567
Skew:                           0.434   Prob(JB):                     3.12e-08
Kurtosis:                       2.772   Cond. No.                     1.23e+04
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
[2] The condition number is large, 1.23e+04. This might indicate that there are
strong multicollinearity or other numerical problems.
                            OLS Regression Results
==============================================================================
Dep. Variable:                  csMPa   R-squared:                       0.028
Model:                            OLS   Adj. R-squared:                  0.027
Method:                 Least Squares   F-statistic:                     29.58
Date:                Fri, 15 Oct 2021   Prob (F-statistic):           6.70e-08
Time:                        16:43:15   Log-Likelihood:                -4346.6
No. Observations:                1030   AIC:                             8697.
Df Residuals:                    1028   BIC:                             8707.
Df Model:                           1
```

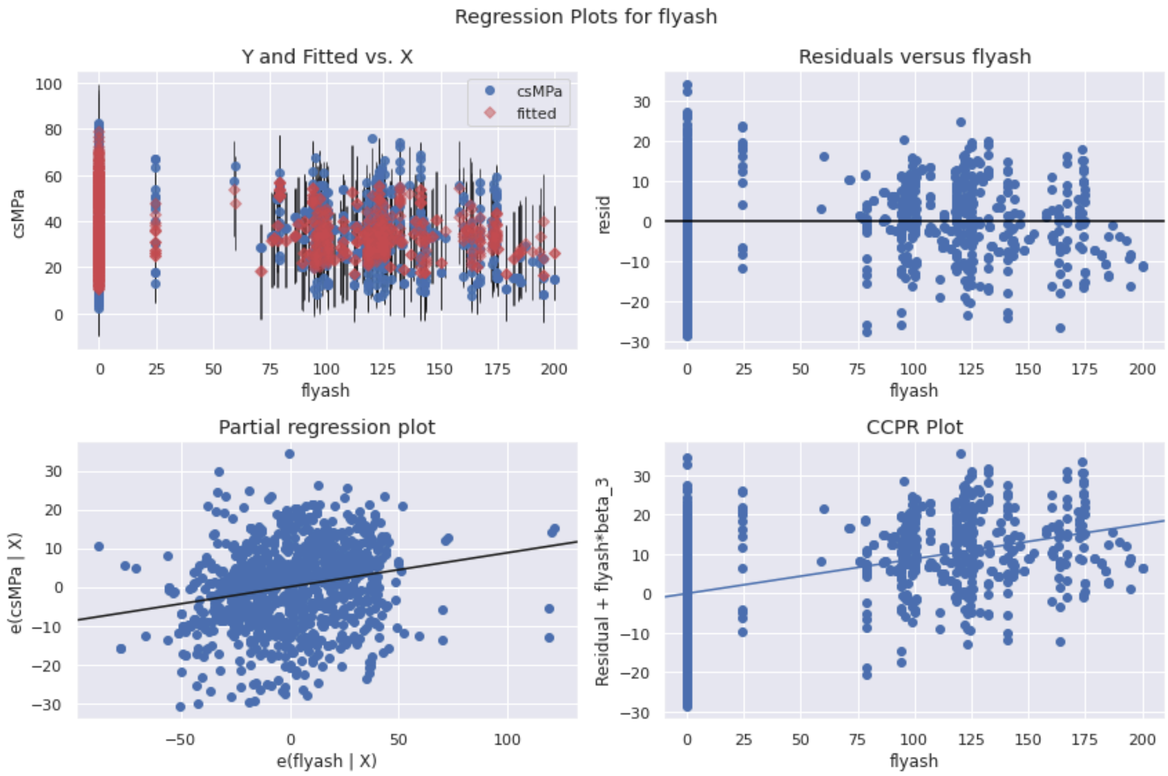
```
Covariance Type:            nonrobust
=================================================================================
                    coef    std err          t      P>|t|      [0.025      0.975]
---------------------------------------------------------------------------------
const            62.7749      4.983     12.598      0.000      52.997      72.553
fineaggregate    -0.0348      0.006     -5.439      0.000      -0.047      -0.022
==============================================================================
Omnibus:                       39.248   Durbin-Watson:                   0.858
Prob(Omnibus):                  0.000   Jarque-Bera (JB):               41.943
Skew:                           0.478   Prob(JB):                     7.80e-10
Kurtosis:                       2.745   Cond. No.                     7.55e+03
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
[2] The condition number is large, 7.55e+03. This might indicate that there are
strong multicollinearity or other numerical problems.
                            OLS Regression Results
==============================================================================
Dep. Variable:                  csMPa   R-squared:                       0.108
Model:                            OLS   Adj. R-squared:                  0.107
Method:                 Least Squares   F-statistic:                     124.7
Date:                Fri, 15 Oct 2021   Prob (F-statistic):           2.11e-27
Time:                        16:43:15   Log-Likelihood:                -4302.3
No. Observations:                1030   AIC:                             8609.
Df Residuals:                    1028   BIC:                             8618.
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const         31.8466      0.607     52.470      0.000      30.656      33.038
age            0.0870      0.008     11.166      0.000       0.072       0.102
==============================================================================
Omnibus:                       46.822   Durbin-Watson:                   0.763
Prob(Omnibus):                  0.000   Jarque-Bera (JB):               52.414
Skew:                           0.548   Prob(JB):                     4.15e-12
Kurtosis:                       2.859   Cond. No.                         96.2
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
```

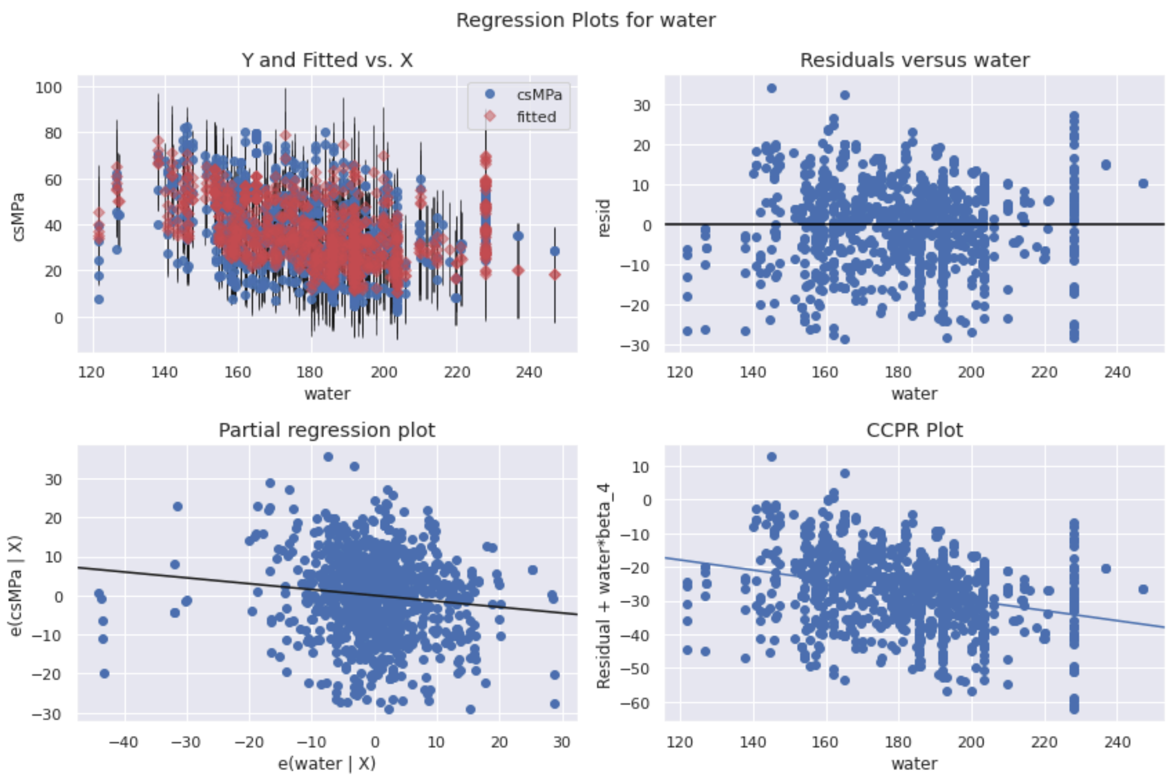
In [25]:

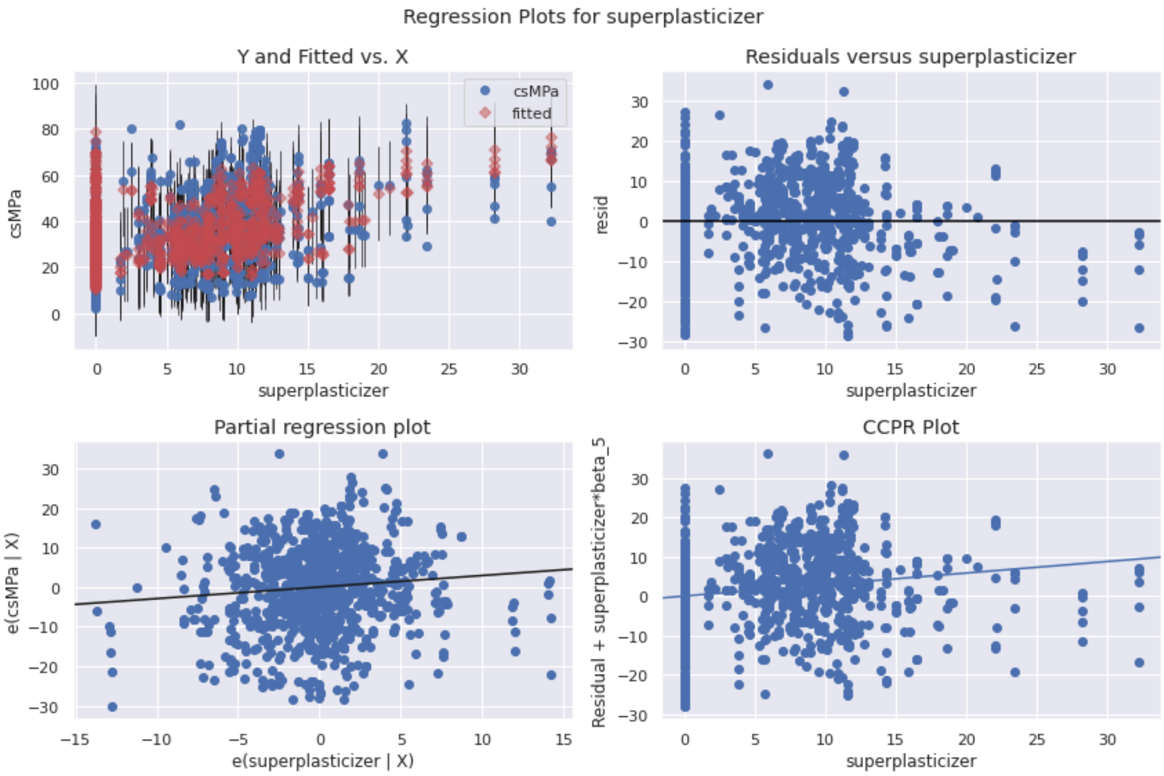
```python
from statsmodels.formula.api import ols

#fit multiple linear regression model
model = ols('csMPa ~ cement + slag + flyash + water + superplasticizer + coarsea

#create residual vs. predictor plot for 'assists'
for i in X.columns:
    fig = plt.figure(figsize=(12,8))
    fig = sm.graphics.plot_regress_exog(model, i, fig=fig)
    fig.show()
```

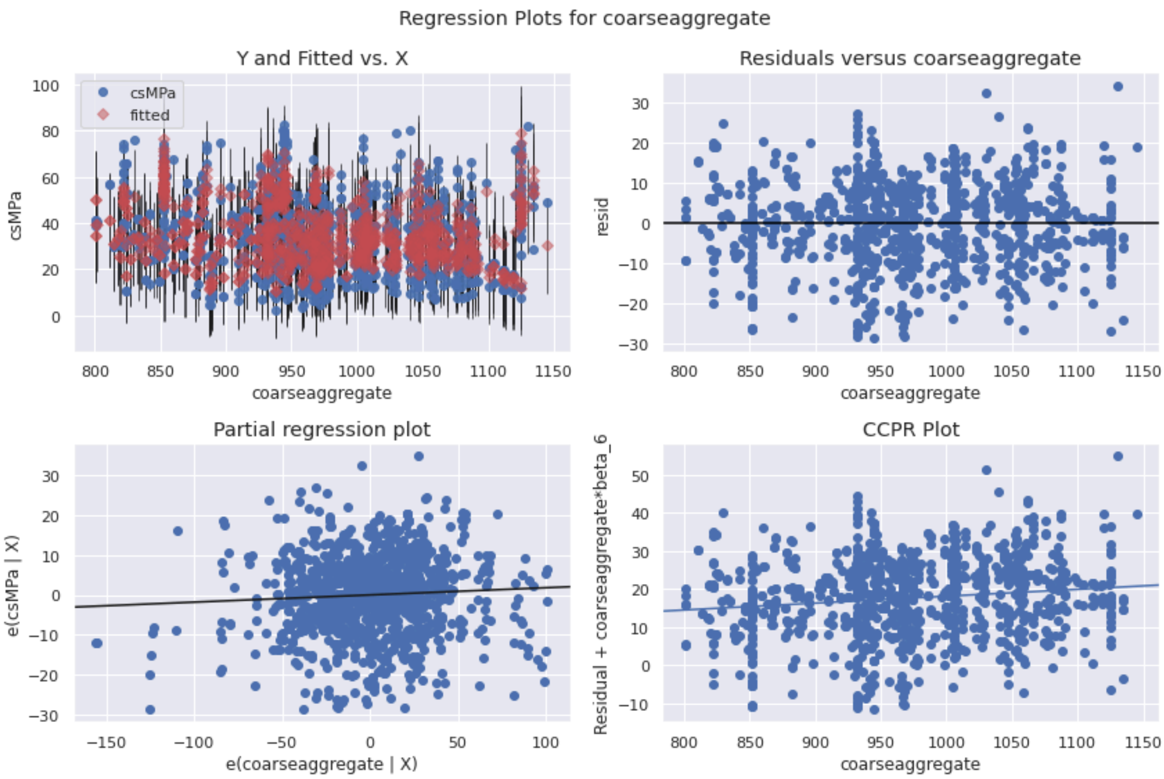

Regression Plots for cement
Y and Fitted vs. X
csMPa
fitted
cement
Residuals versus cement
resid
Partial regression plot
e(csMPa | X)
e(cement | X)
CCPR Plot
Residual + cement*beta_1

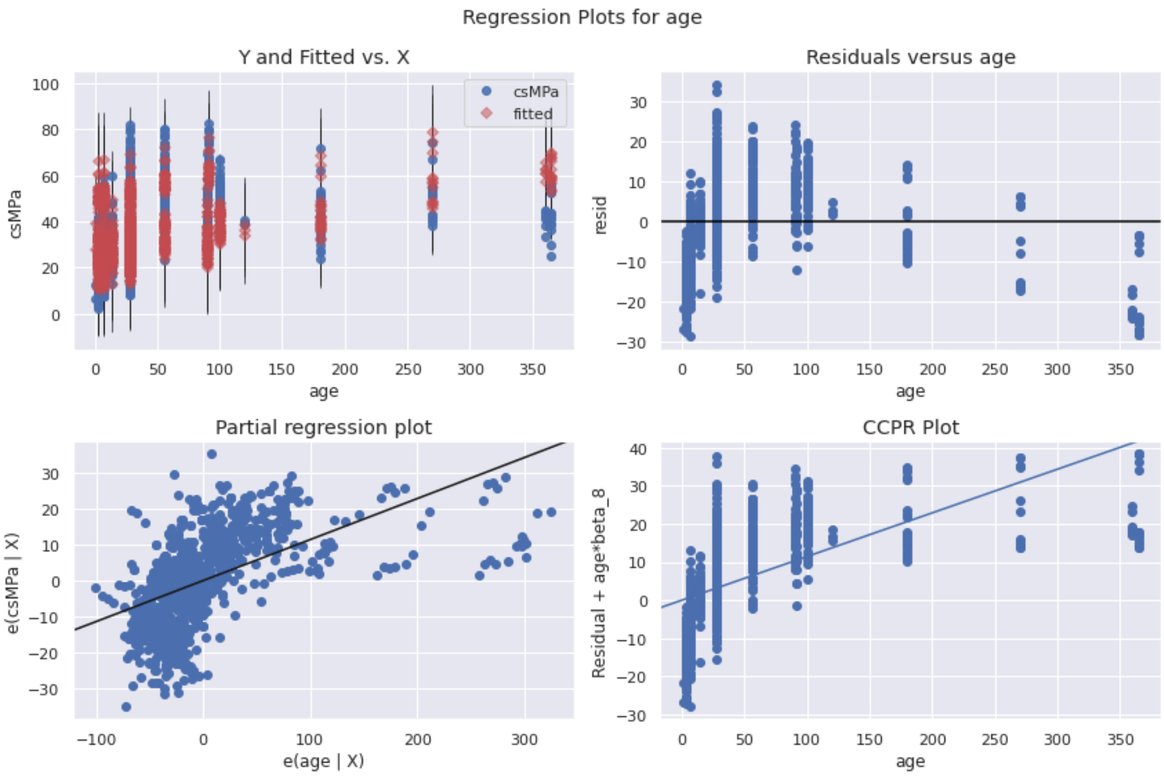

Regression Plots for slag
Y and Fitted vs. X
csMPa
fitted
slag
Residuals versus slag
resid
Partial regression plot
e(csMPa | X)
e(slag | X)
CCPR Plot
Residual + slag*beta_2


Regression Plots for flyash
Y and Fitted vs. X
csMPa
fitted
flyash
Residuals versus flyash
resid
Partial regression plot
e(csMPa | X)
e(flyash | X)
CCPR Plot
Residual + flyash*beta_3


Regression Plots for water
Y and Fitted vs. X
csMPa
fitted
water
Residuals versus water
resid
Partial regression plot
e(csMPa | X)
e(water | X)
CCPR Plot
Residual + water*beta_4


Regression Plots for superplasticizer
Y and Fitted vs. X
csMPa
fitted
superplasticizer
Residuals versus superplasticizer
resid
Partial regression plot
e(csMPa | X)
e(superplasticizer | X)
CCPR Plot
Residual + superplasticizer*beta_5

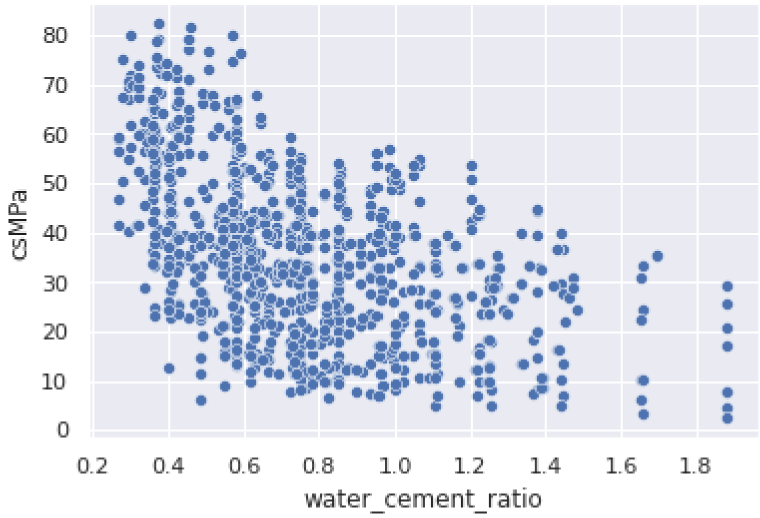

Regression Plots for coarseaggregate
Y and Fitted vs. X
csMPa
fitted
coarseaggregate
Residuals versus coarseaggregate
resid
Partial regression plot
e(csMPa | X)
e(coarseaggregate | X)
CCPR Plot
Residual + coarseaggregate*beta_6



6. Feature Engineering with OLS

In [26]:
```
#feature engineering using knowledge that water:cement ratio is an important fac
X['water_cement_ratio'] = X['water']/X['cement']
```

In [27]:
```
#plot water:cement ratio against compressive strength
sns.scatterplot(x=X['water_cement_ratio'], y=y)
plt.show()
```



In [28]:
```
#generate OLS regression results with water : cement ratio
X_sm = sm.add_constant(X)
model = sm.OLS(y,X_sm)
print(model.fit().summary())
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                  csMPa   R-squared:                       0.618
Model:                            OLS   Adj. R-squared:                  0.615
Method:                 Least Squares   F-statistic:                     183.6
Date:                Fri, 15 Oct 2021   Prob (F-statistic):          2.28e-206
Time:                        16:43:27   Log-Likelihood:                -3865.2
No. Observations:                1030   AIC:                             7750.
Df Residuals:                    1020   BIC:                             7800.
Df Model:                           9
Covariance Type:            nonrobust
=================================================================================
=====
                         coef    std err          t      P>|t|      [0.025
0.975]
---------------------------------------------------------------------------------
-----
const                -16.1769     26.631     -0.607      0.544     -68.434      3
6.080
cement                 0.1013      0.011      9.346      0.000       0.080
0.123
slag                   0.1062      0.010     10.473      0.000       0.086
0.126
flyash                 0.0881      0.013      7.023      0.000       0.063
0.113
water                 -0.1226      0.041     -2.971      0.003      -0.204      -
0.042
superplasticizer       0.2893      0.093      3.106      0.002       0.107
0.472
coarseaggregate        0.0164      0.009      1.750      0.081      -0.002
0.035
fineaggregate          0.0204      0.011      1.908      0.057      -0.001
0.041
age                    0.1132      0.005     20.884      0.000       0.103
0.124
water_cement_ratio    -7.3785      2.699     -2.734      0.006     -12.675      -
2.082
==============================================================================
Omnibus:                        7.306   Durbin-Watson:                   1.279
Prob(Omnibus):                  0.026   Jarque-Bera (JB):                7.216
Skew:                          -0.199   Prob(JB):                       0.0271
Kurtosis:                       3.097   Cond. No.                     1.07e+05
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly
specified.
[2] The condition number is large, 1.07e+05. This might indicate that there are
strong multicollinearity or other numerical problems.
```

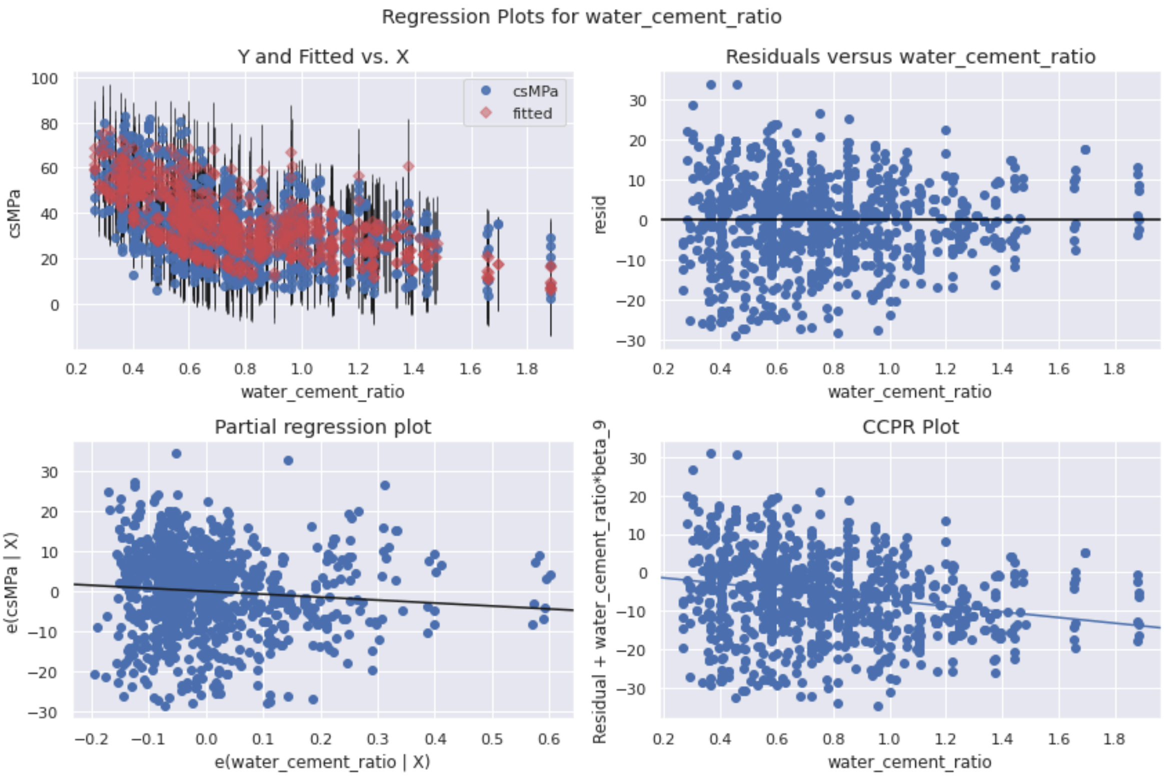
In [29]:

```
#generate OLS summary with only water : cement ratio
X_sm = sm.add_constant(X['water_cement_ratio'])
model = sm.OLS(y,X_sm)
print(model.fit().summary())
```

```
                            OLS Regression Results                            
==============================================================================
Dep. Variable:                  csMPa   R-squared:                       0.251
Model:                            OLS   Adj. R-squared:                  0.250
Method:                 Least Squares   F-statistic:                     343.9
Date:                Fri, 15 Oct 2021   Prob (F-statistic):           1.86e-66
Time:                        16:43:27   Log-Likelihood:                -4212.6
No. Observations:                1030   AIC:                             8429.
Df Residuals:                    1028   BIC:                             8439.
Df Model:                           1                                         
Covariance Type:            nonrobust                                         
==================================================================================
=====
                        coef    std err          t      P>|t|      [0.025      
0.975]
----------------------------------------------------------------------------------
-----
const                55.7502      1.165     47.834      0.000      53.463      5
8.037
water_cement_ratio  -26.6379      1.436    -18.545      0.000     -29.456     -2
3.819
==============================================================================
Omnibus:                       29.143   Durbin-Watson:                   1.022
Prob(Omnibus):                  0.000   Jarque-Bera (JB):               17.972
Skew:                           0.176   Prob(JB):                     0.000125
Kurtosis:                       2.456   Cond. No.                         5.09
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly 
specified.
```

Looking at the p-value of the t-statistic: water : cement ratio has a strong association with compressive strength.

In [30]:
```
#copy water : cement ratio into concrete data
concrete_data['water_cement_ratio'] = X['water_cement_ratio']

#fit multiple linear regression model with water : cement ratio
model = ols('csMPa ~ cement + slag + flyash + water + superplasticizer + coarsea

#plot regression plots for water : cement ratio
fig = plt.figure(figsize=(12,8))
fig = sm.graphics.plot_regress_exog(model, 'water_cement_ratio', fig=fig)
fig.show()
```



Water : cement ratio residuals exhibits a near linear relationship.

7. Preparing Data for ML

In [31]:
```
#import ML preprocessing packages
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler
```

In [32]:
```
#column names
feature_names = X.columns

#train/test split 75% training, 25% test
X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=0.75, randc

#numerical pipeline
scaler=MinMaxScaler()

#apply scaler to numerical data
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)
```

8. ML Baselines

In [33]:
```
#import ML packages
from sklearn.linear_model import LinearRegression
from sklearn.ensemble import RandomForestRegressor, GradientBoostingRegressor
from xgboost import XGBRegressor
from sklearn.model_selection import cross_val_score
from numpy import mean
from numpy import std
```

In [34]:
```
#LinearRegression mean cross-validation
lm = LinearRegression()
lm.fit(X_train, y_train)
cv = cross_val_score(lm,X_train,y_train,scoring='neg_mean_absolute_error',cv=5)
print('LinearRegression')
print(mean(cv), '+/-', std(cv))
```

```
LinearRegression
-8.07027940327449 +/- 0.9042563541306468
```

In [35]:
```
#RandomForestRegressor mean cross-validation
rf = RandomForestRegressor(random_state = 1)
cv = cross_val_score(rf,X_train,y_train,scoring='neg_mean_absolute_error',cv=5)
print('RandomForestRegressor')
print(mean(cv), '+/-', std(cv))
```

```
RandomForestRegressor
-3.741303784820554 +/- 0.1746349225638862
```

In [36]:
```
#GradientBoostingRegressor mean cross-validation
gbr = GradientBoostingRegressor(random_state = 1)
cv = cross_val_score(gbr,X_train,y_train,scoring='neg_mean_absolute_error',cv=5)
print('GradientBoostingRegressor')
print(mean(cv), '+/-', std(cv))
```

```
GradientBoostingRegressor
-3.8930976574254514 +/- 0.14455688824589297
```

In [37]:
```
#XGBoost mean cross-validation
xgb = XGBRegressor(random_state = 1)
cv = cross_val_score(xgb,X_train,y_train,scoring='neg_mean_absolute_error',cv=5)
print('XGBoost')
print(mean(cv), '+/-', std(cv))
```

```
XGBoost
-3.149192175484103 +/- 0.17553754090972187
```

9. Hyperparameter Tuning

In [38]:
```
#ml algorithm tuner
from sklearn.model_selection import GridSearchCV

#performance reporting function
def clf_performance(regressor, model_name):
    print(model_name)
    print('Best Score: {} +/- {}'.format(str(regressor.best_score_),str(regresso
    print('Best Parameters: ' + str(regressor.best_params_))
```

In [39]:
```
#LinearRegression GridSearchCV
lm = LinearRegression()
param_grid = {
                'fit_intercept':[True,False],
                'normalize':[True,False],
                'copy_X':[True, False]
}
clf_lm = GridSearchCV(lm, param_grid = param_grid, cv = 5, scoring='neg_mean_abs
best_clf_lm = clf_lm.fit(X_train,y_train)
clf_performance(best_clf_lm,'LinearRegressor')
```

```
LinearRegressor
Best Score: -8.060702077432467 +/- 0.8846924722871585
Best Parameters: {'copy_X': True, 'fit_intercept': False, 'normalize': True}
```

In [40]:
```
#RanddomForestRegressor GridSearchCV
rf = RandomForestRegressor(random_state = 1)
param_grid = {
                'n_estimators': np.arange(160,200,2) ,
                'bootstrap': [True,False],
#                 'max_depth': [20,30,40],
#                 'max_features': ['auto','sqrt','log2'],
#                  'min_samples_leaf': [2],
#                  'min_samples_split': [6,8,10]
              }
clf_rf = GridSearchCV(rf, param_grid = param_grid, cv = 5, scoring='neg_mean_abs
best_clf_rf = clf_rf.fit(X_train,y_train)
clf_performance(best_clf_rf,'RandomForestRegressor')
```

```
RandomForestRegressor
Best Score: -3.752174984879036 +/- 0.16962584492518898
Best Parameters: {'bootstrap': True, 'n_estimators': 192}
```

In [41]:
```
#GradientBoostingRegressor GridSearchCV
gbr = GradientBoostingRegressor(random_state = 1)
param_grid = {
                'n_estimators': [160],
                'max_depth': [4],
                'max_features': ['auto'],
                'learning_rate': np.arange(.1,1,.1),
                'alpha': [0.0001],
                'min_samples_leaf': [2],
                'min_samples_split': np.arange(2,6,1)
              }
clf_gbr = GridSearchCV(gbr, param_grid = param_grid, cv = 5, scoring='neg_mean_a
best_clf_gbr = clf_gbr.fit(X_train,y_train)
clf_performance(best_clf_gbr,'GradientBoostingRegressor')
```

```
GradientBoostingRegressor
Best Score: -3.0637915704624037 +/- 0.17629198413614053
Best Parameters: {'alpha': 0.0001, 'learning_rate': 0.2, 'max_depth': 4, 'max_fea
tures': 'auto', 'min_samples_leaf': 2, 'min_samples_split': 2, 'n_estimators': 16
0}
```

In [42]:
```
#XGBoost GridSearchCV
xgb = XGBRegressor(random_state = 1)
param_grid = {
#               'nthread':[4],
#               'objective':['reg:linear'],
#               'learning_rate': [0.3],
              'max_depth': [4],
#               'min_child_weight': [1],
#               'subsample': [1],
#               'colsample_bytree': np.arange(0.5,1,0.1),
              'n_estimators': [500]
              }
clf_xgb = GridSearchCV(xgb, param_grid = param_grid, cv = 5, scoring='neg_mean_a
best_clf_xgb = clf_xgb.fit(X_train,y_train)
clf_performance(best_clf_xgb,'XGBoost')
```

```
XGBoost
Best Score: -3.020177287831604 +/- 0.18068834764455305
Best Parameters: {'max_depth': 4, 'n_estimators': 500}
```

10. Assessing Models

In [43]:
```
#import metrics packages
from sklearn.metrics import mean_squared_error, mean_absolute_error, r2_score
```

In [44]:
```
#GradientBoostingRegressor metrics
gbr = GradientBoostingRegressor(alpha = 0.0001,
                                learning_rate= 0.2,
                                max_depth= 4,
                                max_features='auto',
                                min_samples_leaf= 2,
                                min_samples_split= 2,
                                n_estimators= 160,
                                random_state = 1)
gbr.fit(X_train,y_train)
tpred_gbr=gbr.predict(X_test)
print('GradientBoostingRegressor')
print('MSE: {}'.format(mean_squared_error(y_test,tpred_gbr)))
print('RMSE: {}'.format(np.sqrt(mean_squared_error(y_test,tpred_gbr))))
print('MAE: {}'.format(mean_absolute_error(y_test,tpred_gbr)))
print('R-squared: {}'.format(r2_score(y_test,tpred_gbr)))
```

```
GradientBoostingRegressor
MSE: 19.928264399385675
RMSE: 4.464108466355368
MAE: 3.0586929775691822
R-squared: 0.9252890876328432
```

In [45]:
```
#XGBoost metrics
xgb = XGBRegressor(max_depth=4,
                   n_estimators=500,
                   random_state = 1)
xgb.fit(X_train,y_train)
tpred_xgb=xgb.predict(X_test)
print('XGBoost')
print('MSE: {}'.format(mean_squared_error(y_test,tpred_xgb)))
print('RMSE: {}'.format(np.sqrt(mean_squared_error(y_test,tpred_xgb))))
print('MAE: {}'.format(mean_absolute_error(y_test,tpred_xgb)))
print('R-squared: {}'.format(r2_score(y_test,tpred_xgb)))
```

```
XGBoost
MSE: 17.557246580616614
RMSE: 4.190136821228707
MAE: 2.824839199236197
R-squared: 0.9341780154857116
```

11. Feature Importance

In [46]:
```
#import packages for explaining feature importance
import eli5
from eli5.sklearn import PermutationImportance
```

In [47]:
```
#permutation importance from xgboost
perm = PermutationImportance(xgb).fit(X_test, y_test)
eli5.show_weights(perm, feature_names = list(feature_names), top=len(feature_nam
```

Out[47]:

Weight	Feature
0.9126 ± 0.1335	age
0.4932 ± 0.0844	water_cement_ratio
0.1878 ± 0.0439	slag
0.1332 ± 0.0161	water
0.0837 ± 0.0158	fineaggregate
0.0426 ± 0.0082	coarseaggregate
0.0396 ± 0.0058	superplasticizer
0.0365 ± 0.0022	cement
0.0085 ± 0.0030	flyash