2020_1125_Comparison_with_Linear_Models

November 25, 2020

1 Predicting Concrete Compressive Strength - Comparison with Linear Models

In this code notebook, we will analyze the statistics pertaining the various models presented in this project. In the Exploratory Data Analysis notebook, we explored the various relationships that each consituent of concrete has on the cured compressive strength. The materials that held the strongest relationships, regardless of curing time, were cement, cementitious ratio, superplasticizer ratio, and fly ash ratio. We will examine each of the linear ratios independent of age, as well as at the industry-standard 28 day cure time mark.

1.1 Dataset Citation

This dataset was retrieved from the UC Irvine Machine Learning Repository from the following URL: https://archive.ics.uci.edu/ml/datasets/Concrete+Compressive+Strength.

The dataset was donated to the UCI Repository by Prof. I-Cheng Yeh of Chung-Huah University, who retains copyright for the following published paper: I-Cheng Yeh, "Modeling of strength of high performance concrete using artificial neural networks," Cement and Concrete Research, Vol. 28, No. 12, pp. 1797-1808 (1998). Additional papers citing this dataset are listed at the reference link above.

1.2 Import the Relevant Libraries

[1]:
```
# Data Manipulation
import numpy as np
import pandas as pd

# Data Visualization
import matplotlib.pyplot as plt
import seaborn as sns
%matplotlib inline
sns.set()

# Data Preprocessing
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler

# Linear Regresssion Model
```

```python
from sklearn.linear_model import LinearRegression

# Model Evaluation
from sklearn.metrics import␣
 ↪mean_squared_error,mean_absolute_error,explained_variance_score
```

1.3 Import & Check the Data

[2]:
```python
df1 = pd.read_csv('2020_1124_Modeling_Data.csv')
df2 = pd.read_csv('2020_1123_Concrete_Data_Loaded_Transformed.csv')

original_data = df1.copy()
transformed_data = df2.copy()
```

[3]:
```python
# The original data contains kg/m^3 values
original_data.head()
```

[3]:
```
   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  Compressive_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
```

[4]:
```python
# Original data
original_data.describe()
```

[4]:
```
            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

       Compressive_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
```

[5]:
```
# The transformed data contains ratios to total mass of the concrete mix
transformed_data.head()
```

[5]:
```
   Cementitious_Ratio  Slag_Ratio  Fly_Ash_Ratio  Water_to_Cementitious_Ratio  \
0            0.205086    0.000000            0.0                     0.400000
1            0.167391    0.000000            0.0                     0.483117
2            0.058291    0.087436            0.0                     1.375358
3            0.145726    0.000000            0.0                     0.550143
4            0.085350    0.056900            0.0                     0.966767

   Superplasticizer_Ratio  Coarse_Aggregate_Ratio  Sand_Ratio  Age  \
0                     0.0                0.461444    0.251436    1
1                     0.0                0.420000    0.331739    1
2                     0.0                0.437179    0.336924    3
3                     0.0                0.437179    0.336924    3
4                     0.0                0.420474    0.354764    3

   Compressive_Strength
0             12.638095
1              6.267337
2              8.063422
3             15.049193
4              9.131420
```

[6]:
```
# Transformed data
transformed_data.describe()
```

[6]:
```
       Cementitious_Ratio   Slag_Ratio  Fly_Ash_Ratio  \
count         1030.000000  1030.000000    1030.000000
mean             0.142726     0.031643       0.155263
```

```
std                0.040513     0.036961       0.187884
min                0.044815     0.000000       0.000000
25%                0.124002     0.000000       0.000000
50%                0.143272     0.009455       0.000000
75%                0.162794     0.061972       0.319960
max                0.259517     0.150339       0.588415

       Water_to_Cementitious_Ratio  Superplasticizer_Ratio  \
count                  1030.000000             1030.000000
mean                      0.611796                0.002620
std                       0.278319                0.002494
min                       0.265918                0.000000
25%                       0.447540                0.000000
50%                       0.547837                0.002727
75%                       0.666639                0.004338
max                       1.882353                0.013149

       Coarse_Aggregate_Ratio   Sand_Ratio          Age  Compressive_Strength
count             1030.000000  1030.000000  1030.000000           1030.000000
mean                 0.415166     0.330117    45.662136             35.817836
std                  0.031021     0.033245    63.169912             16.705679
min                  0.345890     0.247971     1.000000              2.331808
25%                  0.392294     0.311208     7.000000             23.707115
50%                  0.420464     0.330543    28.000000             34.442774
75%                  0.437623     0.354096    56.000000             46.136287
max                  0.479846     0.414147   365.000000             82.599225
```

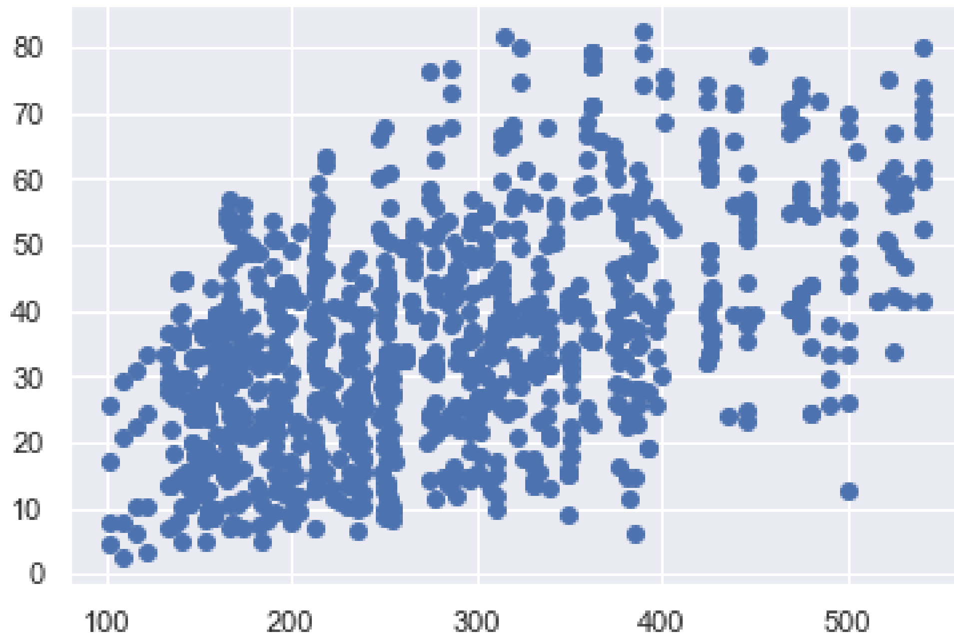
1.4 Cement Modeling - Including All Cure Times

We understand that the ratio of cement to compressive strength is linear. We will model this relationship in Python and evaluate its performance compared to our ANN model.

1.4.1 Visualization

[7]:
```python
# We will visualize the linear relationship between quantity of cement and compressive strength
cement = original_data['Cement']
strength = original_data['Compressive_Strength']
plt.scatter(cement,strength)
```

[7]:
```
<matplotlib.collections.PathCollection at 0x7ff55c9991c0>
```



1.4.2 Train the Linear Model

[8]:
```
# Reshape the data so it complies with the linear model requirements
X = np.array(cement).reshape(1030,1)
y = np.array(strength).reshape(1030,1)
```

[9]:
```
# Perform a train-test split
X_train, X_test, y_train, y_test = train_test_split(X,y,test_size=0.
↪2,random_state=42)

# Train the linear model
lm = LinearRegression()
lm.fit(X_train,y_train)
```

[9]:
```
LinearRegression()
```

1.4.3 Test the Linear Model

[10]:
```
y_pred = lm.predict(X_test)
```

1.4.4 Linear Equation

[11]:
```
# print the intercept
print(lm.intercept_)
```

```
[13.78517188]
```

[12]:
```
coeff = pd.DataFrame(lm.coef_,columns=['Coefficient'])
coeff
```

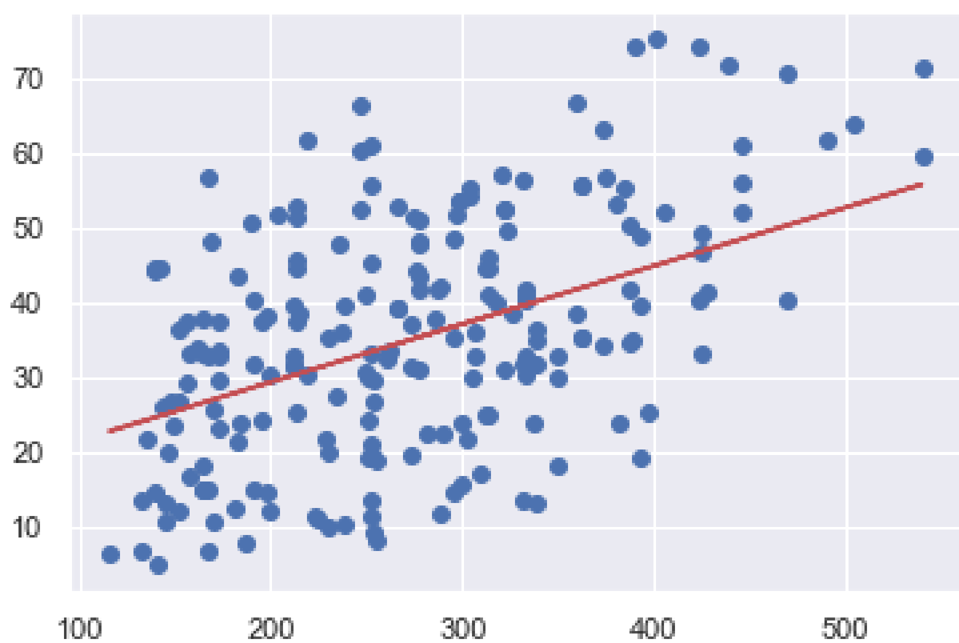
[12]:

	Coefficient
0	0.077896

1.4.5 Model Evaluation

[13]:
```
# Plot the linear model preditions as a line superimposed on a scatter plot of␣
↪the testing data
plt.scatter(X_test,y_test)
plt.plot(X_test,y_pred,'r')
```

[13]: [<matplotlib.lines.Line2D at 0x7ff55cd19760>]



[14]:
```
# Evaluation Metrics
MAE_cement = mean_absolute_error(y_test, y_pred)
MSE_cement = mean_squared_error(y_test, y_pred)
RMSE_cement = np.sqrt(mean_squared_error(y_test, y_pred))
```

```
cement_stats = [MAE_cement,MSE_cement,RMSE_cement] # storing for model␣
↪comparison at the end of this notebook

# Print the metrics
print(f"EVALUATION METRICS, LINEAR MODEL FOR CEMENT VS. COMPRESSIVE STRENGTH")
print('-----------------------------')
print(f"Mean Absolute Error (MAE):\t\t{MAE_cement}\nMean Squared Error:
↪\t\t\t{MSE_cement}\nRoot Mean Squared Error (RMSE):\t\t{RMSE_cement}")
print('-----------------------------\n\n')
```

```
EVALUATION METRICS, LINEAR MODEL FOR CEMENT VS. COMPRESSIVE STRENGTH
-----------------------------
Mean Absolute Error (MAE):              11.55561279863471
Mean Squared Error:                     192.78479855432548
Root Mean Squared Error (RMSE):         13.884696559677689
-----------------------------
```

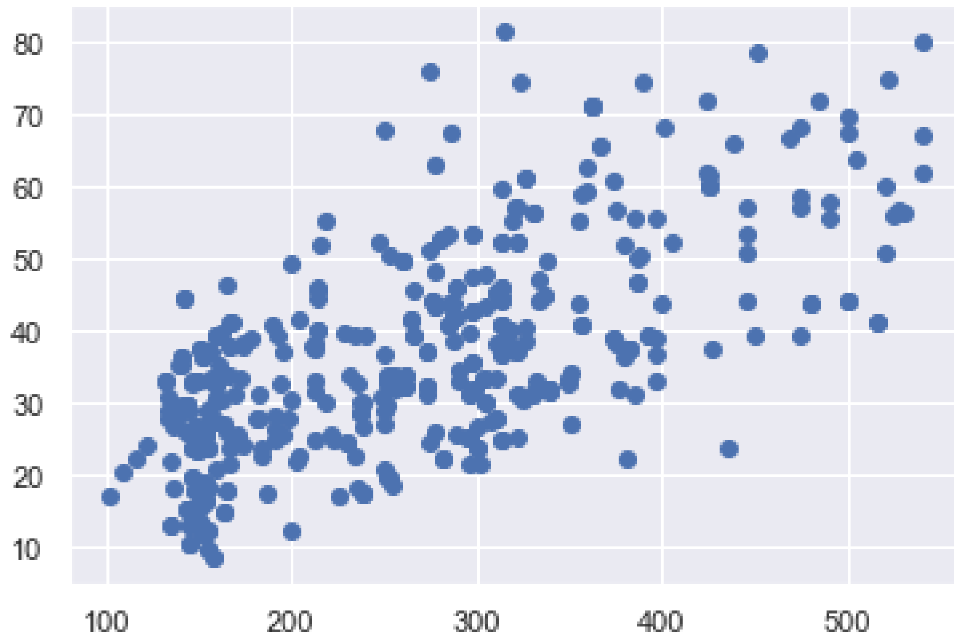
1.5 Cement Modeling - 28 Day Cure Time

We will model the cement vs compressive strength relationship for a constant cure time (28 days).

1.5.1 Visualization

[15]:
```
# We will visualize the linear relationship between quantity of cement and␣
↪compressive strength at 28 days
cement = original_data[original_data['Age']==28]['Cement']
strength = original_data[original_data['Age']==28]['Compressive_Strength']
plt.scatter(cement,strength)
```

[15]:
```
<matplotlib.collections.PathCollection at 0x7ff55cd70d90>
```



1.5.2 Train the Linear Model

[16]:
```
# Reshape the data so it complies with the linear model requirements
X = np.array(cement).reshape(425,1)
y = np.array(strength).reshape(425,1)
```

[17]:
```
# Perform a train-test split
X_train, X_test, y_train, y_test = train_test_split(X,y,test_size=0.
↪2,random_state=42)

# Train the linear model
lm = LinearRegression()
lm.fit(X_train,y_train)
```

[17]:
```
LinearRegression()
```

1.5.3 Test the Linear Model

[18]:
```
y_pred = lm.predict(X_test)
```

1.5.4 Linear Equation

[19]:
```
# print the intercept
print(lm.intercept_)
```

```
[13.07410297]
```

[20]:
```
coeff = pd.DataFrame(lm.coef_,columns=['Coefficient'])
coeff
```

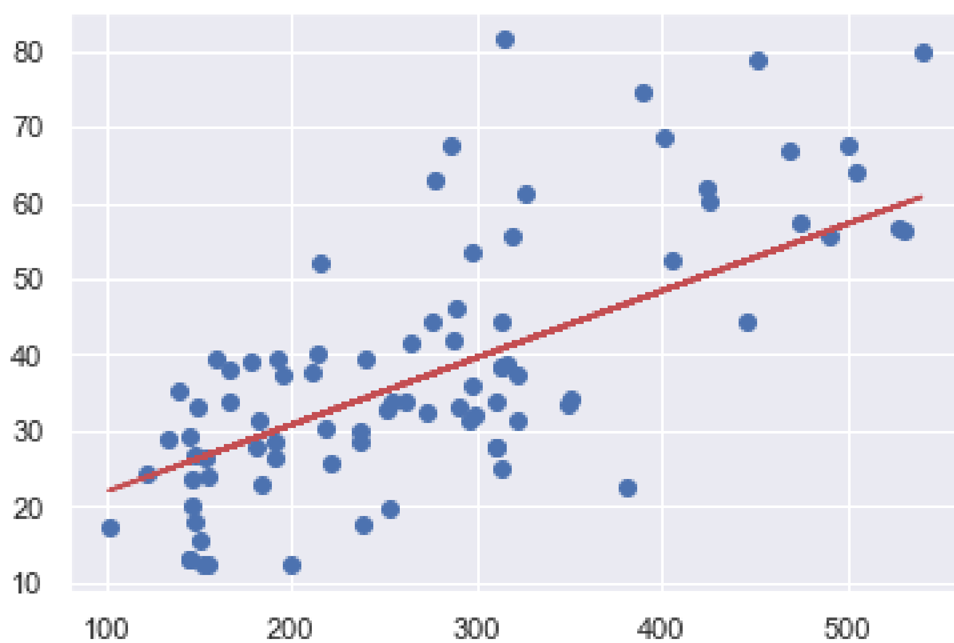
[20]:

	Coefficient
0	0.088248

1.5.5 Model Evaluation

[21]:
```
# Plot the linear model preditions as a line superimposed on a scatter plot of␣
↪the testing data
plt.scatter(X_test,y_test)
plt.plot(X_test,y_pred,'r')
```

[21]: [<matplotlib.lines.Line2D at 0x7ff55dbb01f0>]



[22]:
```
# Evaluation Metrics
MAE_cement_28 = mean_absolute_error(y_test, y_pred)
MSE_cement_28 = mean_squared_error(y_test, y_pred)
RMSE_cement_28 = np.sqrt(mean_squared_error(y_test, y_pred))
```

```
cement_28_stats = [MAE_cement_28,MSE_cement_28,RMSE_cement_28] # storing for␣
↪model comparison at the end of this notebook

# Print the metrics
print(f"EVALUATION METRICS, LINEAR MODEL FOR CEMENT VS. COMPRESSIVE STRENGTH")
print('-----------------------------')
print(f"Mean Absolute Error (MAE):\t\t{MAE_cement_28}\nMean Squared Error:
↪\t\t\t{MSE_cement_28}\nRoot Mean Squared Error (RMSE):\t\t{RMSE_cement_28}")
print('-----------------------------\n\n')
```

```
EVALUATION METRICS, LINEAR MODEL FOR CEMENT VS. COMPRESSIVE STRENGTH
-----------------------------
Mean Absolute Error (MAE):              9.134081632197555
Mean Squared Error:                     140.11750347700305
Root Mean Squared Error (RMSE):         11.837123952928899
-----------------------------
```

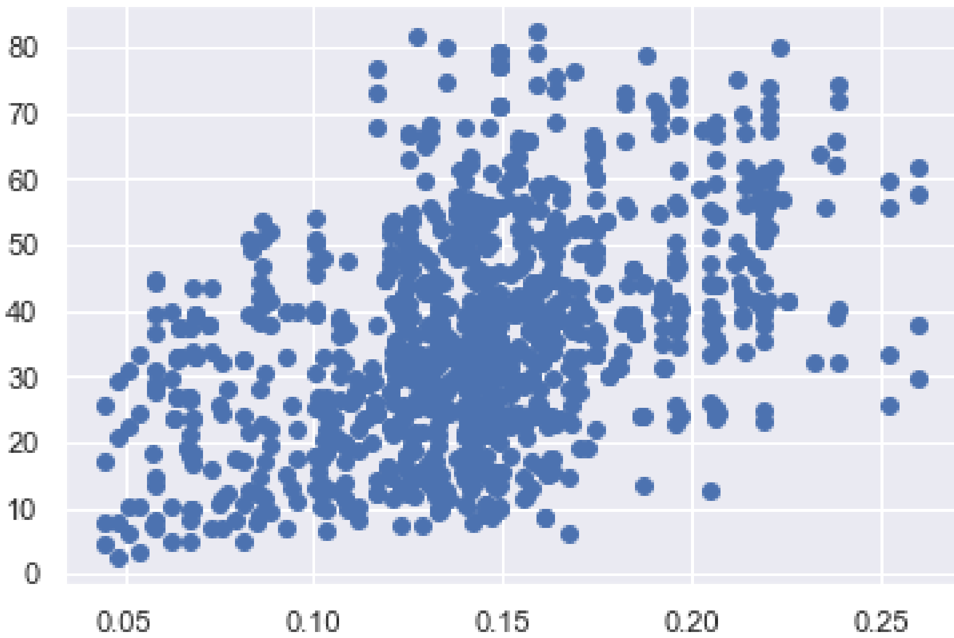
1.6 Cementitious Ratio Modeling - Including All Cure Times

We know that the ratio of cementitious materials to the total mass is (cement + fly ash)/(total mass) to compressive strength is linear. We will model this relationship in Python and evaluate its performance.

1.6.1 Visualization

[23]:
```
# We will visualize the linear relationship between quantity of cementitious␣
↪materials and compressive strength
cementitious = transformed_data['Cementitious_Ratio']
strength = transformed_data['Compressive_Strength']
plt.scatter(cementitious,strength)
```

[23]:
```
<matplotlib.collections.PathCollection at 0x7ff55dbe5c10>
```



1.6.2 Train the Linear Model

[24]:
```
# Reshape the data so it complies with the linear model requirements
X = np.array(cementitious).reshape(1030,1)
y = np.array(strength).reshape(1030,1)
```

[25]:
```
# Perform a train-test split
X_train, X_test, y_train, y_test = train_test_split(X,y,test_size=0.
 ↪2,random_state=42)

# Train the linear model
lm = LinearRegression()
lm.fit(X_train,y_train)
```

[25]: LinearRegression()

1.6.3 Test the Linear Model

[26]:
```
y_pred = lm.predict(X_test)
```

1.6.4 Linear Equation

[27]:
```
# print the intercept
print(lm.intercept_)
```

```
[10.00280955]
```

[28]:
```
coeff = pd.DataFrame(lm.coef_,columns=['Coefficient'])
coeff
```

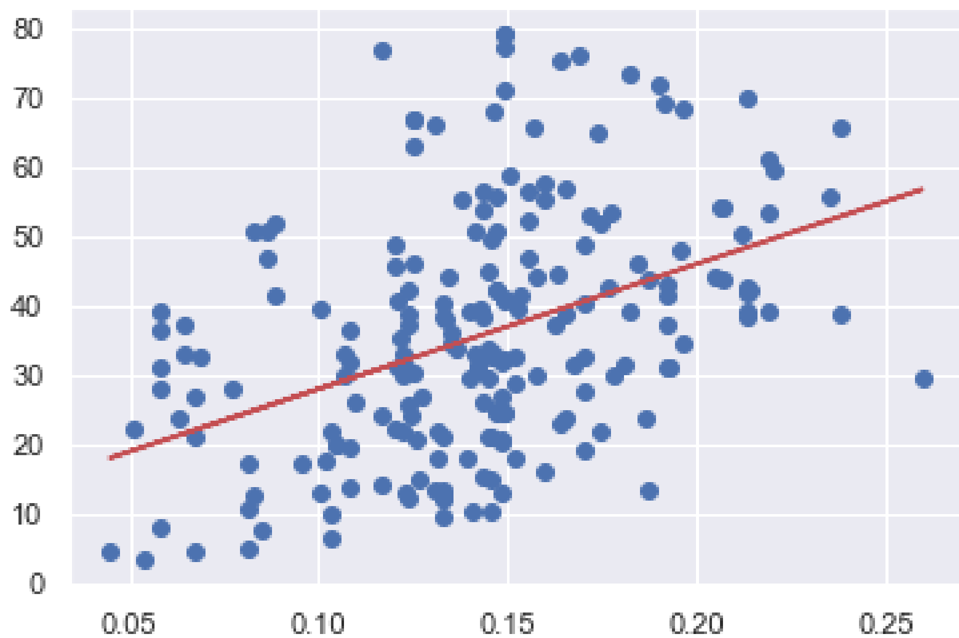
[28]:

	Coefficient
0	180.19044

1.6.5 Model Evaluation

[29]:
```
# Plot the linear model preditions as a line superimposed on a scatter plot of␣
↪the testing data
plt.scatter(X_test,y_test)
plt.plot(X_test,y_pred,'r')
```

[29]:
```
[<matplotlib.lines.Line2D at 0x7ff55dd229a0>]
```



[30]:
```
# Evaluation Metrics
MAE_cementitious = mean_absolute_error(y_test, y_pred)
MSE_cementitious = mean_squared_error(y_test, y_pred)
RMSE_cementitious = np.sqrt(mean_squared_error(y_test, y_pred))
```

```
cementitious_stats = [MAE_cementitious,MSE_cementitious,RMSE_cementitious] #␣
↪storing for model comparison at the end of this notebook

# Print the metrics
print(f"EVALUATION METRICS, LINEAR MODEL FOR CEMENTITIOUS RATIO VS. COMPRESSIVE␣
↪STRENGTH")
print('-----------------------------')
print(f"Mean Absolute Error (MAE):\t\t{MAE_cementitious}\nMean Squared Error:
↪\t\t\t{MSE_cementitious}\nRoot Mean Squared Error (RMSE):
↪\t\t{RMSE_cementitious}")
print('-----------------------------\n\n')
```

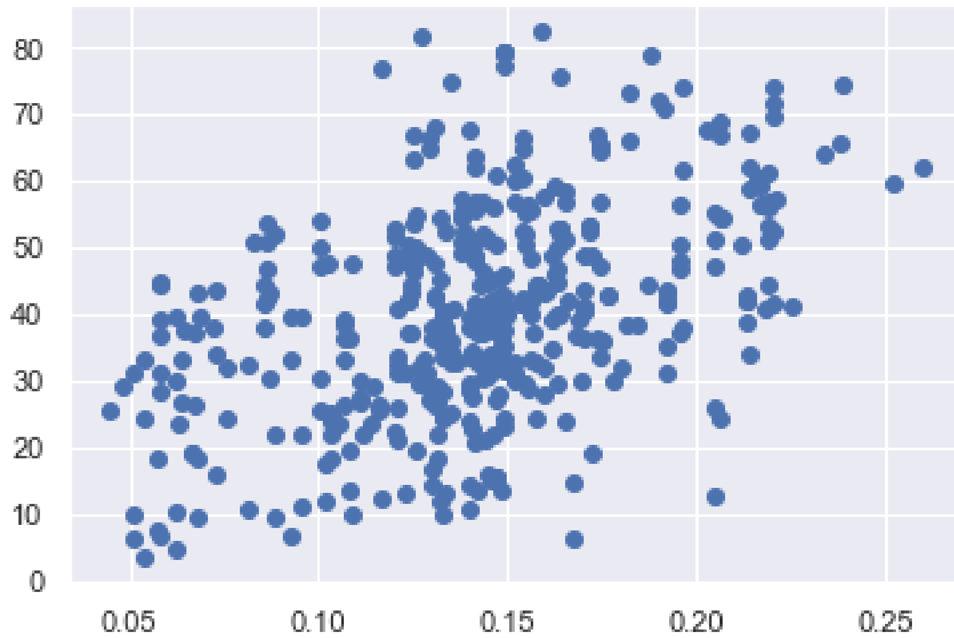
```
EVALUATION METRICS, LINEAR MODEL FOR CEMENTITIOUS RATIO VS. COMPRESSIVE STRENGTH
-----------------------------
Mean Absolute Error (MAE):          12.834672509172698
Mean Squared Error:                 253.05814774985234
Root Mean Squared Error (RMSE):     15.907801474429217
-----------------------------
```

1.7 Cementitious Ratio Modeling - 28 Day Cure Time

1.7.1 Visualization

[31]:
```
# We will visualize the linear relationship between quantity of cementitious␣
↪materials and compressive strength at 28 days
cementitious = transformed_data[original_data['Age']==28]['Cementitious_Ratio']
strength = transformed_data[original_data['Age']==28]['Compressive_Strength']
plt.scatter(cementitious,strength)
```

[31]:
```
<matplotlib.collections.PathCollection at 0x7ff55de47fa0>
```



1.7.2 Train the Linear Model

[32]:
```
# Reshape the data so it complies with the linear model requirements
X = np.array(cementitious).reshape(425,1)
y = np.array(strength).reshape(425,1)
```

[33]:
```
# Perform a train-test split
X_train, X_test, y_train, y_test = train_test_split(X,y,test_size=0.
 ↪2,random_state=42)

# Train the linear model
lm = LinearRegression()
lm.fit(X_train,y_train)
```

[33]:
```
LinearRegression()
```

1.7.3 Test the Linear Model

[34]:
```
y_pred = lm.predict(X_test)
```

1.7.4 Linear Equation

[35]:
```python
# print the intercept
print(lm.intercept_)
```

```
[13.59333113]
```

[36]:
```python
coeff = pd.DataFrame(lm.coef_,columns=['Coefficient'])
coeff
```

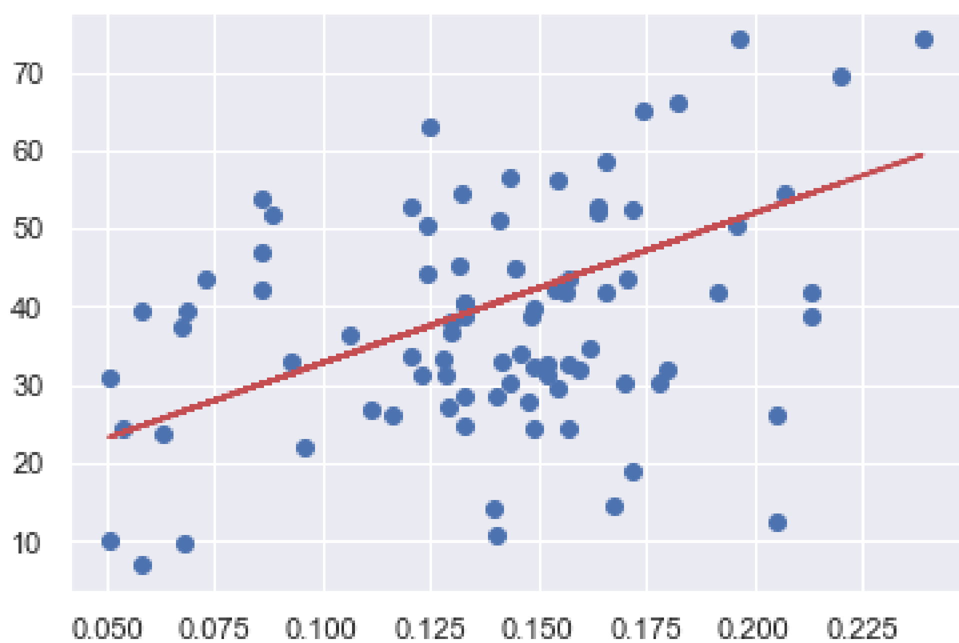
[36]:

	Coefficient
0	191.571248

1.7.5 Model Evaluation

[37]:
```python
# Plot the linear model preditions as a line superimposed on a scatter plot of␣
↪the testing data
plt.scatter(X_test,y_test)
plt.plot(X_test,y_pred,'r')
```

[37]: [<matplotlib.lines.Line2D at 0x7ff55deaa880>]



[38]:
```python
# Evaluation Metrics
MAE_cementitious_28 = mean_absolute_error(y_test, y_pred)
MSE_cementitious_28 = mean_squared_error(y_test, y_pred)
RMSE_cementitious_28 = np.sqrt(mean_squared_error(y_test, y_pred))
```

```
cementitious_28_stats =
↪[MAE_cementitious_28,MSE_cementitious_28,RMSE_cementitious_28] # storing for
↪model comparison at the end of this notebook

# Print the metrics
print(f"EVALUATION METRICS, LINEAR MODEL FOR CEMENTITIOUS RATIO VS. COMPRESSIVE
↪STRENGTH AT 28 DAYS")
print('-----------------------------')
print(f"Mean Absolute Error (MAE):\t\t{MAE_cementitious_28}\nMean Squared Error:
↪\t\t\t{MSE_cementitious_28}\nRoot Mean Squared Error (RMSE):
↪\t\t{RMSE_cementitious_28}")
print('-----------------------------\n\n')
```

```
EVALUATION METRICS, LINEAR MODEL FOR CEMENTITIOUS RATIO VS. COMPRESSIVE STRENGTH
AT 28 DAYS
-----------------------------
Mean Absolute Error (MAE):              11.519580245958837
Mean Squared Error:                     197.95720060481753
Root Mean Squared Error (RMSE):         14.069726386991949
-----------------------------
```

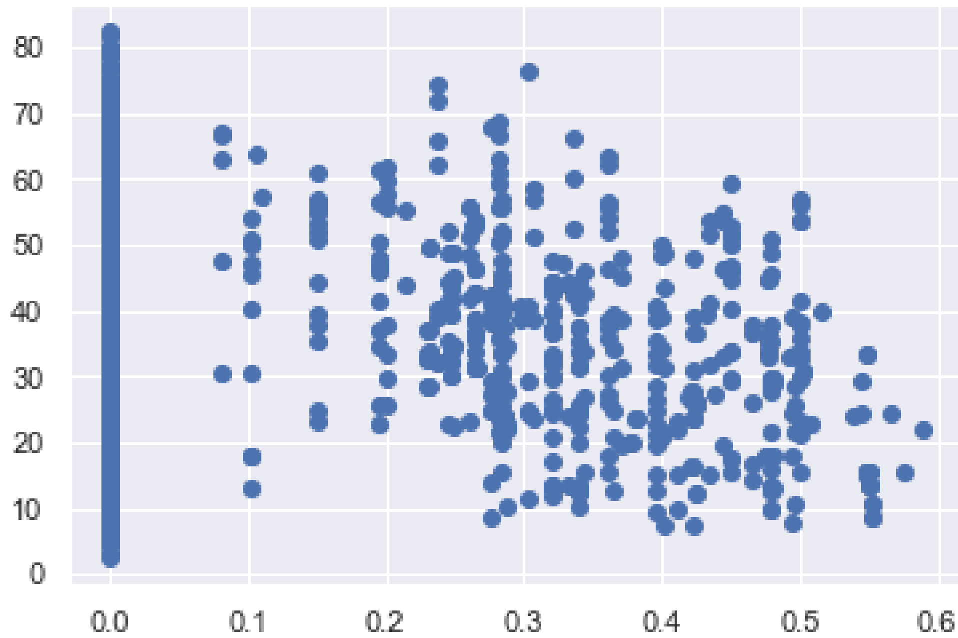
1.8 Fly Ash Ratio Modeling - Including All Cure Times

The fly ash ratio is interpreted as the percentage of fly ash within the cementitious materials mix, that is, Fly_Ash_Ratio = (fly ash + cement)/(total mass).

1.8.1 Visualization

[39]:
```
# We will visualize the linear relationship between fly ash ratio and
↪compressive strength
fly = transformed_data['Fly_Ash_Ratio']
strength = transformed_data['Compressive_Strength']
plt.scatter(fly,strength)
```

[39]: <matplotlib.collections.PathCollection at 0x7ff55db156a0>

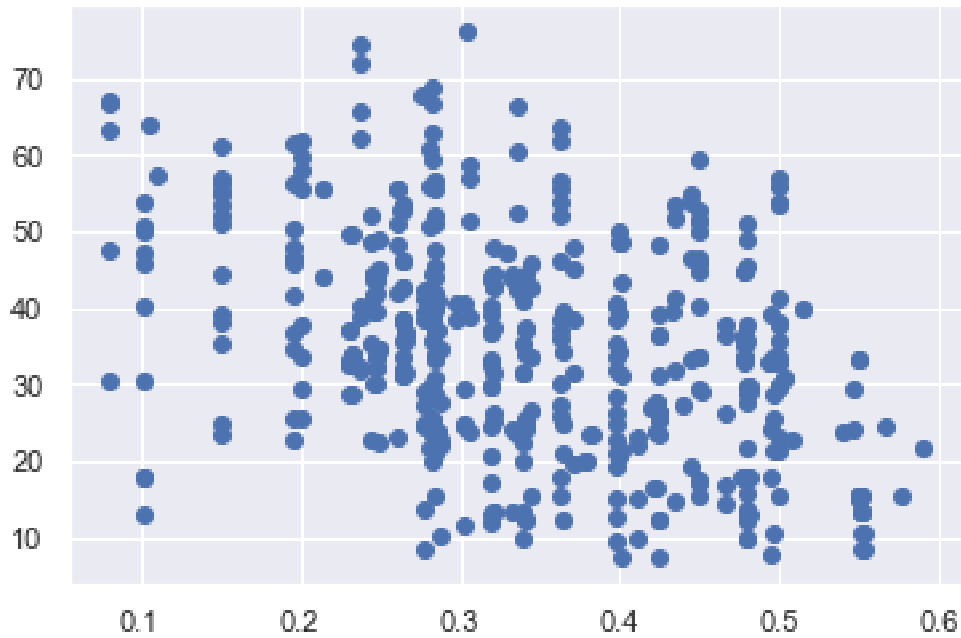


1.8.2 Data Preprocessing

We see from the graph above that there are many instances where there is no fly ash in the mix design. Let us use only nonzero entries for our analysis.

[40]:
```
fly = transformed_data[transformed_data['Fly_Ash_Ratio']!=0]['Fly_Ash_Ratio']
strength = transformed_data[transformed_data['Fly_Ash_Ratio']!
 ↪=0]['Compressive_Strength']
plt.scatter(fly,strength)
```

[40]: <matplotlib.collections.PathCollection at 0x7ff5600d4a60>



1.8.3 Train the Linear Model

[41]:
```
# Reshape the data so it complies with the linear model requirements
X = np.array(fly).reshape(464,1)
y = np.array(strength).reshape(464,1)
```

[42]:
```
# Perform a train-test split
X_train, X_test, y_train, y_test = train_test_split(X,y,test_size=0.
↪2,random_state=42)

# Train the linear model
lm = LinearRegression()
lm.fit(X_train,y_train)
```

[42]:
```
LinearRegression()
```

1.8.4 Test the Linear Model

[43]:
```
y_pred = lm.predict(X_test)
```

1.8.5 Linear Equation

[44]:
```
# print the intercept
print(lm.intercept_)
```

```
[53.13047155]
```

[45]:
```
coeff = pd.DataFrame(lm.coef_,columns=['Coefficient'])
coeff
```

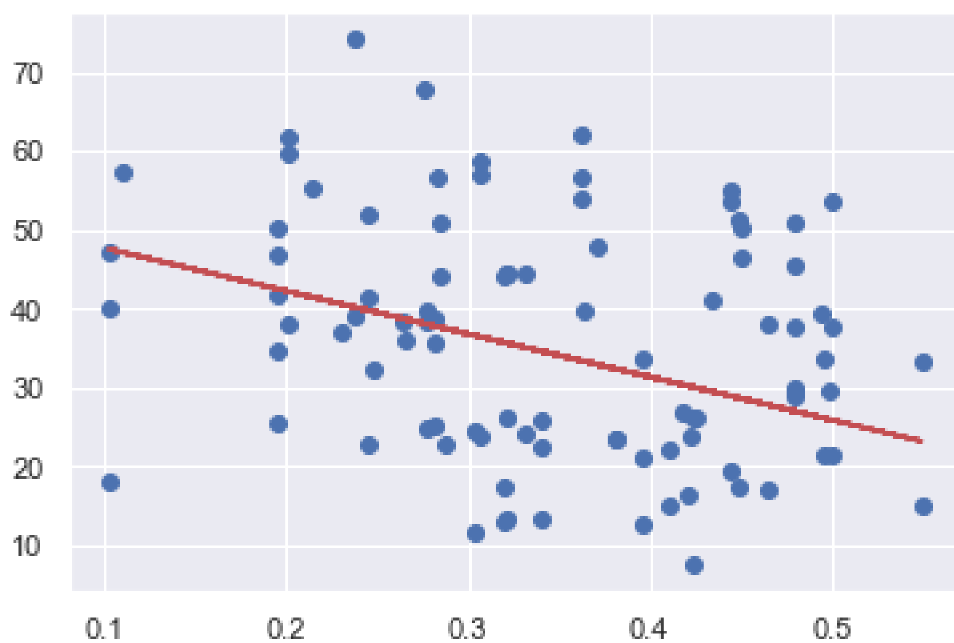
[45]:

	Coefficient
0	-54.508785

1.8.6 Model Evaluation

[46]:
```
# Plot the linear model preditions as a line superimposed on a scatter plot of␣
↪the testing data
plt.scatter(X_test,y_test)
plt.plot(X_test,y_pred,'r')
```

[46]:
```
[<matplotlib.lines.Line2D at 0x7ff56012ddc0>]
```



[47]:
```
# Evaluation Metrics
MAE_fly = mean_absolute_error(y_test, y_pred)
MSE_fly = mean_squared_error(y_test, y_pred)
RMSE_fly = np.sqrt(mean_squared_error(y_test, y_pred))
```

```
fly_stats = [MAE_fly,MSE_fly,RMSE_fly] # storing for model comparison at the␣
↪end of this notebook

# Print the metrics
print(f"EVALUATION METRICS, LINEAR MODEL FOR FLY ASH RATIO VS. COMPRESSIVE␣
↪STRENGTH")
print('-----------------------------')
print(f"Mean Absolute Error (MAE):\t\t{MAE_fly}\nMean Squared Error:
↪\t\t\t{MSE_fly}\nRoot Mean Squared Error (RMSE):\t\t{RMSE_fly}")
print('-----------------------------\n\n')
```

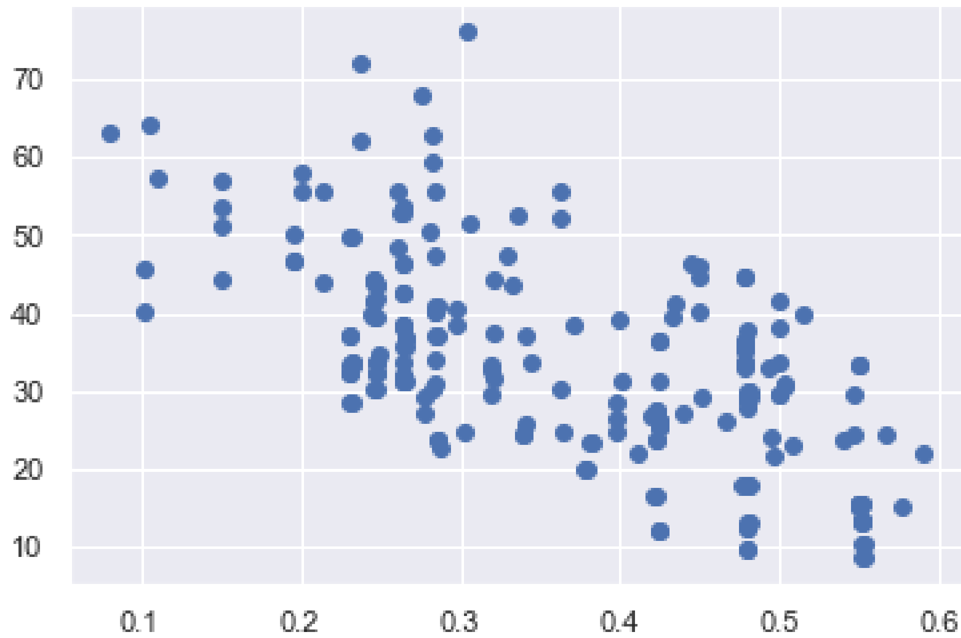
```
EVALUATION METRICS, LINEAR MODEL FOR FLY ASH RATIO VS. COMPRESSIVE STRENGTH
-----------------------------
Mean Absolute Error (MAE):          12.121987321537818
Mean Squared Error:                 212.8943249027957
Root Mean Squared Error (RMSE):     14.590898700998363
-----------------------------
```

1.9 Fly Ash Ratio Modeling - 28 Day Cure Time

The fly ash ratio is interpreted as the percentage of fly ash within the cementitious materials mix, that is, Fly_Ash_Ratio = (fly ash + cement)/(total mass).

[48]:
```
fly = transformed_data[((transformed_data['Fly_Ash_Ratio']!
↪=0)&(transformed_data['Age']==28))]['Fly_Ash_Ratio']
strength = transformed_data[((transformed_data['Fly_Ash_Ratio']!
↪=0)&(transformed_data['Age']==28))]['Compressive_Strength']
plt.scatter(fly,strength)
```

[48]:
```
<matplotlib.collections.PathCollection at 0x7ff5601eac40>
```



1.9.1 Train the Linear Model

[49]:
```
# Reshape the data so it complies with the linear model requirements
X = np.array(fly).reshape(217,1)
y = np.array(strength).reshape(217,1)
```

[50]:
```
# Perform a train-test split
X_train, X_test, y_train, y_test = train_test_split(X,y,test_size=0.
 ↪2,random_state=42)

# Train the linear model
lm = LinearRegression()
lm.fit(X_train,y_train)
```

[50]:
```
LinearRegression()
```

1.9.2 Test the Linear Model

[51]:
```
y_pred = lm.predict(X_test)
```

1.9.3 Linear Equation

[52]:
```
# print the intercept
print(lm.intercept_)
```

```
[60.04189914]
```

[53]:
```
coeff = pd.DataFrame(lm.coef_,columns=['Coefficient'])
coeff
```

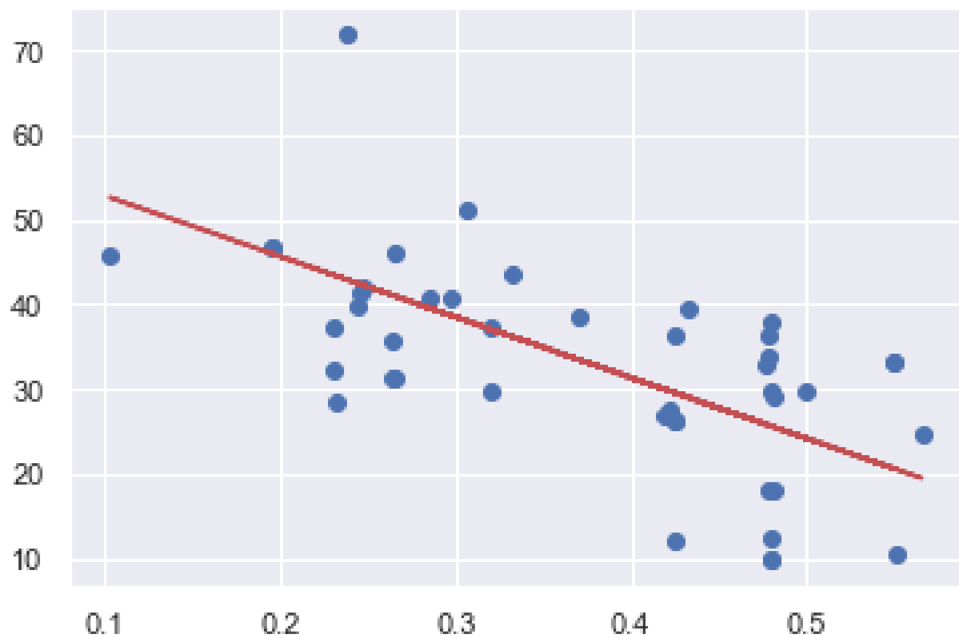
[53]:

	Coefficient
0	-71.730364

1.9.4 Model Evaluation

[54]:
```
# Plot the linear model preditions as a line superimposed on a scatter plot of␣
↪the testing data
plt.scatter(X_test,y_test)
plt.plot(X_test,y_pred,'r')
```

[54]: [<matplotlib.lines.Line2D at 0x7ff56036bd00>]



[55]:
```
# Evaluation Metrics
MAE_fly_28 = mean_absolute_error(y_test, y_pred)
MSE_fly_28 = mean_squared_error(y_test, y_pred)
RMSE_fly_28 = np.sqrt(mean_squared_error(y_test, y_pred))
```

```
fly_28_stats = [MAE_fly_28,MSE_fly_28,RMSE_fly_28] # storing for model␣
↪comparison at the end of this notebook

# Print the metrics
print(f"EVALUATION METRICS, LINEAR MODEL FOR FLY ASH RATIO VS. COMPRESSIVE␣
↪STRENGTH AT 28 DAYS")
print('-----------------------------')
print(f"Mean Absolute Error (MAE):\t\t{MAE_fly_28}\nMean Squared Error:
↪\t\t\t{MSE_fly_28}\nRoot Mean Squared Error (RMSE):\t\t{RMSE_fly_28}")
print('-----------------------------\n\n')
```

```
EVALUATION METRICS, LINEAR MODEL FOR FLY ASH RATIO VS. COMPRESSIVE STRENGTH AT
28 DAYS
-----------------------------
Mean Absolute Error (MAE):              7.692694771235926
Mean Squared Error:                     91.3179595195656
Root Mean Squared Error (RMSE):         9.556043089038768
-----------------------------
```

1.10 Superplasticizer Ratio Modeling - Including All Cure Times

The superplasticizer ratio is the ratio of superplasticizer contained within the total mix design, by weight.

1.10.1 Visualization

[56]:
```
# We will visualize the linear relationship between superplasticizer ratio and␣
↪compressive strength
superplasticizer = transformed_data['Superplasticizer_Ratio']
strength = transformed_data['Compressive_Strength']
plt.scatter(superplasticizer,strength)
```

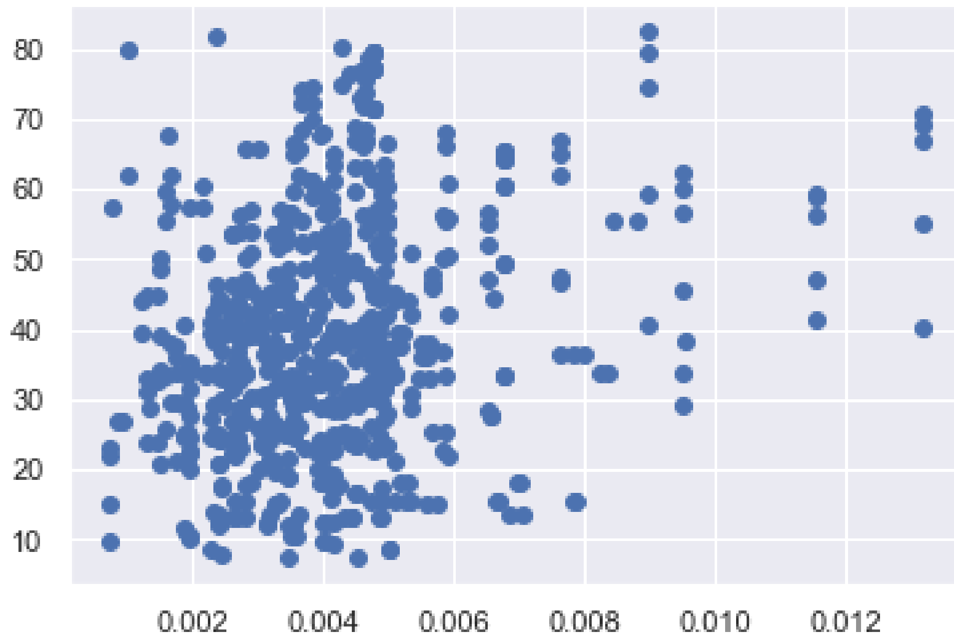
[56]: <matplotlib.collections.PathCollection at 0x7ff5603c2310>

1.10.2 Data Preprocessing

Once agaain, we see from the graph above that there are many instances where there is no superplasticizer in the mix design. Let us use only nonzero entries for our analysis.

[57]:
```
superplasticizer = transformed_data[transformed_data['Superplasticizer_Ratio']!
 ↪=0]['Superplasticizer_Ratio']
strength = transformed_data[transformed_data['Superplasticizer_Ratio']!
 ↪=0]['Compressive_Strength']
plt.scatter(superplasticizer,strength)
```

[57]: <matplotlib.collections.PathCollection at 0x7ff560526130>



This is better, but we see a large spread in the data. Let's remove any outliers first, before training our model.

[58]:
```
superplasticizer.describe()
```

[58]:
```
count    651.000000
mean       0.004146
std        0.001875
min        0.000746
25%        0.002947
50%        0.003998
75%        0.004834
max        0.013149
Name: Superplasticizer_Ratio, dtype: float64
```

[59]:
```
mean = 0.004146
three_sigma = 3*0.001875
upper = mean + three_sigma
lower = mean - three_sigma

print(f"The lower bound is:\t{lower}\nThe upper bound is:\t{upper}")
```

```
The lower bound is:     -0.0014789999999999994
The upper bound is:     0.009771
```

Since there are no negative ratios, we only need to remove data points where the superplasticizer ratio is greater than 0.009771.

[60]:
```
superplasticizer = transformed_data[transformed_data['Superplasticizer_Ratio']!
↪=0][transformed_data['Superplasticizer_Ratio'] <␣
↪upper]['Superplasticizer_Ratio']
strength = transformed_data[transformed_data['Superplasticizer_Ratio']!
↪=0][transformed_data['Superplasticizer_Ratio'] <␣
↪upper]['Compressive_Strength']
plt.scatter(superplasticizer,strength)
```

```
<ipython-input-60-1ad850f1b580>:1: UserWarning: Boolean Series key will be
reindexed to match DataFrame index.
  superplasticizer = transformed_data[transformed_data['Superplasticizer_Ratio']
!=0][transformed_data['Superplasticizer_Ratio'] <
upper]['Superplasticizer_Ratio']
<ipython-input-60-1ad850f1b580>:2: UserWarning: Boolean Series key will be
reindexed to match DataFrame index.
  strength = transformed_data[transformed_data['Superplasticizer_Ratio']!=0][tra
nsformed_data['Superplasticizer_Ratio'] < upper]['Compressive_Strength']
```

[60]:
```
<matplotlib.collections.PathCollection at 0x7ff5606067c0>
```

1.10.3 Train the Linear Model

[61]:
```
# We will train and test our model only on the data above, that does not␣
↪contain outliers
# Reshape the data so it complies with the linear model requirements
```

```
X = np.array(superplasticizer).reshape(641,1)
y = np.array(strength).reshape(641,1)
```

[62]:
```
# Perform a train-test split
X_train, X_test, y_train, y_test = train_test_split(X,y,test_size=0.
 ↪2,random_state=42)

# Train the linear model
lm = LinearRegression()
lm.fit(X_train,y_train)
```

[62]:
```
LinearRegression()
```

1.10.4 Test the Linear Model

[63]:
```
y_pred = lm.predict(X_test)
```

1.10.5 Linear Equation

[64]:
```
# print the intercept
print(lm.intercept_)
```

```
[30.85660295]
```

[65]:
```
coeff = pd.DataFrame(lm.coef_,columns=['Coefficient'])
coeff
```

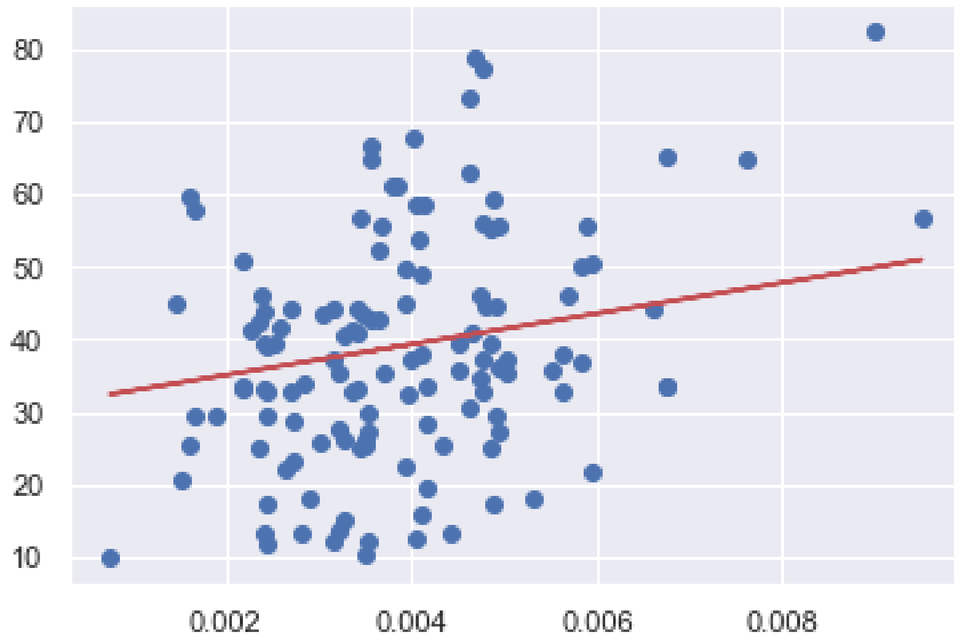
[65]:

	Coefficient
0	2121.483927

1.10.6 Model Evaluation

[66]:
```
# Plot the linear model preditions as a line superimposed on a scatter plot of␣
 ↪the testing data
plt.scatter(X_test,y_test)
plt.plot(X_test,y_pred,'r')
```

[66]:
```
[<matplotlib.lines.Line2D at 0x7ff560663250>]
```



[67]:
```
# Evaluation Metrics
MAE_super = mean_absolute_error(y_test, y_pred)
MSE_super = mean_squared_error(y_test, y_pred)
RMSE_super = np.sqrt(mean_squared_error(y_test, y_pred))

super_stats = [MAE_super,MSE_super,RMSE_super] # storing for model comparison␣
↪at the end of this notebook

# Print the metrics
print(f"EVALUATION METRICS, LINEAR MODEL FOR SUPERPLASTICIZER RATIO VS.␣
↪COMPRESSIVE STRENGTH")
print('-----------------------------')
print(f"Mean Absolute Error (MAE):\t\t{MAE_super}\nMean Squared Error:
↪\t\t\t{MSE_super}\nRoot Mean Squared Error (RMSE):\t\t{RMSE_super}")
print('-----------------------------\n\n')
```

```
EVALUATION METRICS, LINEAR MODEL FOR SUPERPLASTICIZER RATIO VS. COMPRESSIVE
STRENGTH
-----------------------------
Mean Absolute Error (MAE):              12.189766983759341
Mean Squared Error:                     225.90929843844432
Root Mean Squared Error (RMSE):         15.030279386573103
-----------------------------
```

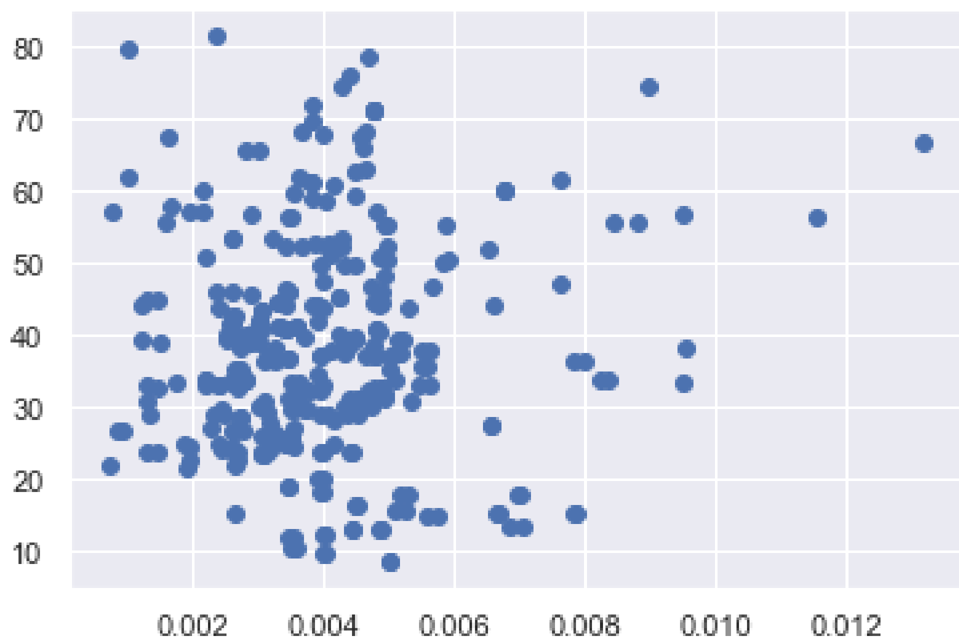
1.11 Superplasticizer Ratio Modeling - 28 Day Cure Time

The superplasticizer ratio is the ratio of superplasticizer contained within the total mix design, by weight.

1.11.1 Visualization

[68]:
```
superplasticizer =␣
↪transformed_data[((transformed_data['Superplasticizer_Ratio']!
↪=0)&(transformed_data['Age']==28))]['Superplasticizer_Ratio']
strength = transformed_data[((transformed_data['Superplasticizer_Ratio']!
↪=0)&(transformed_data['Age']==28))]['Compressive_Strength']
plt.scatter(superplasticizer,strength)
```

[68]:
```
<matplotlib.collections.PathCollection at 0x7ff5606ed580>
```



This is better, but we see a large spread in the data. Let's remove any outliers first, before training our model.

[69]:
```
superplasticizer.describe()
```

[69]:
```
count    317.000000
mean       0.004031
std        0.001713
min        0.000746
25%        0.002988
50%        0.003910
```

```
75%        0.004776
max        0.013149
Name: Superplasticizer_Ratio, dtype: float64
```

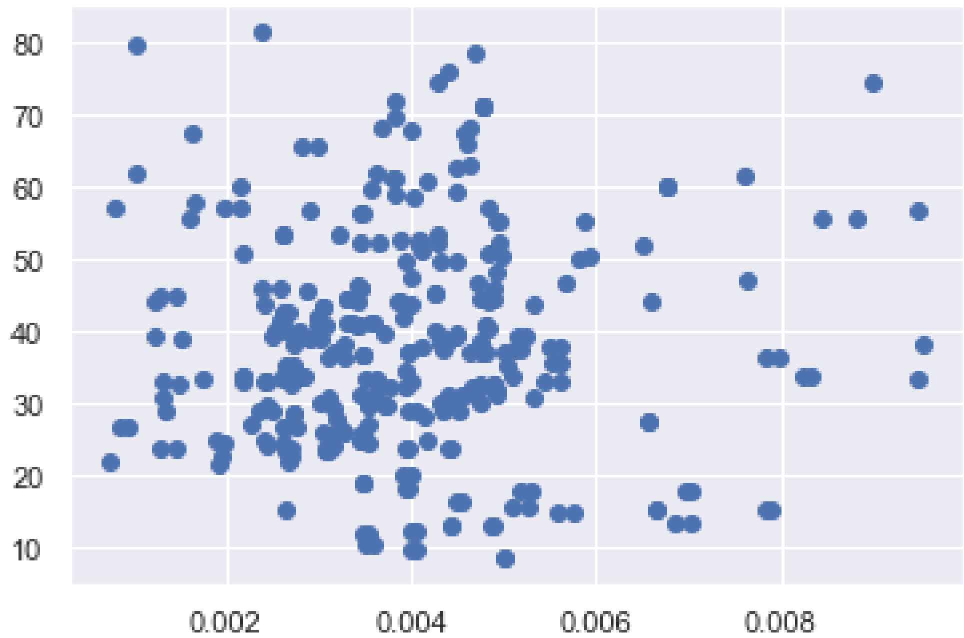
[70]:
```
mean = 0.004146
three_sigma = 3*0.001875
upper = mean + three_sigma
lower = mean - three_sigma

print(f"The lower bound is:\t{lower}\nThe upper bound is:\t{upper}")
```

```
The lower bound is:     -0.0014789999999999994
The upper bound is:     0.009771
```

Since there are no negative ratios, we only need to remove data points where the superplasticizer ratio is greater than 0.009771.

[71]:
```
superplasticizer =␣
↪transformed_data[((transformed_data['Superplasticizer_Ratio']!
↪=0)&(transformed_data['Age']==28)&(transformed_data['Superplasticizer_Ratio']<upper))]['Sup
strength = transformed_data[((transformed_data['Superplasticizer_Ratio']!
↪=0)&(transformed_data['Age']==28)&(transformed_data['Superplasticizer_Ratio']<upper))]['Com
plt.scatter(superplasticizer,strength)
```

[71]: <matplotlib.collections.PathCollection at 0x7ff5607c6730>



1.11.2 Train the Linear Model

[72]:
```
# We will train and test our model only on the data above, that does not␣
↪contain outliers
# Reshape the data so it complies with the linear model requirements
X = np.array(superplasticizer).reshape(315,1)
y = np.array(strength).reshape(315,1)
```

[73]:
```
# Perform a train-test split
X_train, X_test, y_train, y_test = train_test_split(X,y,test_size=0.
↪2,random_state=42)

# Train the linear model
lm = LinearRegression()
lm.fit(X_train,y_train)
```

[73]:
```
LinearRegression()
```

1.11.3 Test the Linear Model

[74]:
```
y_pred = lm.predict(X_test)
```

1.11.4 Linear Equation

[75]:
```
# print the intercept
print(lm.intercept_)
```

```
[36.83431501]
```

[76]:
```
coeff = pd.DataFrame(lm.coef_,columns=['Coefficient'])
coeff
```

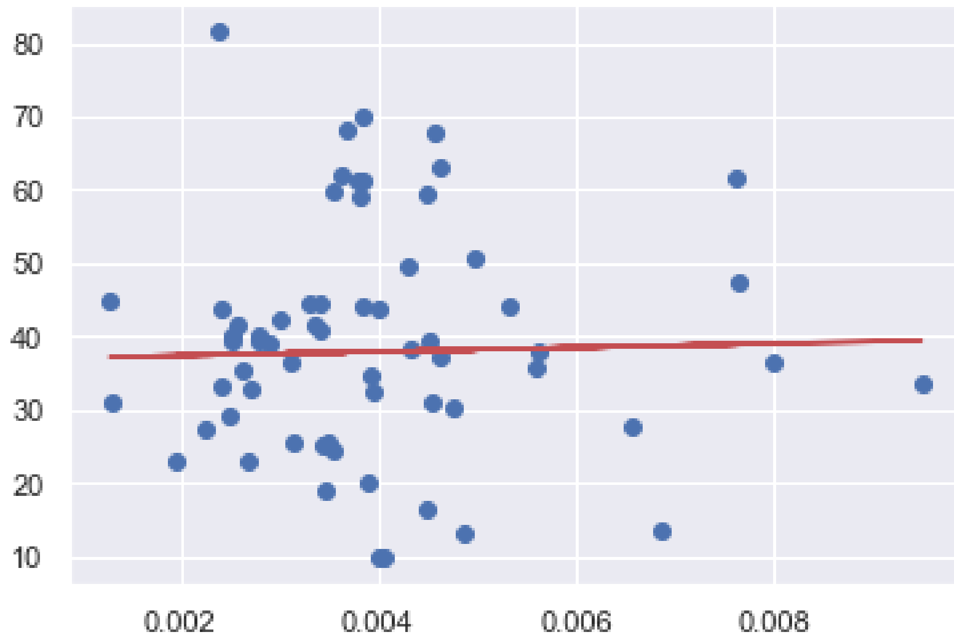
[76]:

	Coefficient
0	273.960172

1.11.5 Model Evaluation

[77]:
```
# Plot the linear model preditions as a line superimposed on a scatter plot of␣
↪the testing data
plt.scatter(X_test,y_test)
plt.plot(X_test,y_pred,'r')
```

[77]:
```
[<matplotlib.lines.Line2D at 0x7ff5608cbe50>]
```



[78]:
```
# Evaluation Metrics
MAE_super_28 = mean_absolute_error(y_test, y_pred)
MSE_super_28 = mean_squared_error(y_test, y_pred)
RMSE_super_28 = np.sqrt(mean_squared_error(y_test, y_pred))

super_stats_28 = [MAE_super_28,MSE_super_28,RMSE_super_28] # storing for model␣
↪comparison at the end of this notebook

# Print the metrics
print(f"EVALUATION METRICS, LINEAR MODEL FOR SUPERPLASTICIZER RATIO VS.␣
↪COMPRESSIVE STRENGTH AT 28 DAYS")
print('-----------------------------')
print(f"Mean Absolute Error (MAE):\t\t{MAE_super_28}\nMean Squared Error:
↪\t\t\t{MSE_super_28}\nRoot Mean Squared Error (RMSE):\t\t{RMSE_super_28}")
print('-----------------------------\n\n')
```

```
EVALUATION METRICS, LINEAR MODEL FOR SUPERPLASTICIZER RATIO VS. COMPRESSIVE
STRENGTH AT 28 DAYS
-----------------------------
Mean Absolute Error (MAE):          11.954354128234902
Mean Squared Error:                 243.9703785891613
Root Mean Squared Error (RMSE):     15.619551164779393
-----------------------------
```

1.12 Model Comparisons Analysis

Neither superplasticizer linear model appeared to represent the data well from a visual perspective. The cement, cementitious ratio, and fly ash ratio linear models, however, did. We can display all of the evaluation metrics below and compare them to the artificial neural network's (ANN) performance.

[103]:
```
ANN_metrics = [5.083552,6.466492**2,6.466492]

metrics = [cement_stats, cementitious_stats, fly_stats, super_stats,␣
↪ANN_metrics]
metrics_28 = [cement_28_stats, cementitious_28_stats, fly_28_stats,␣
↪super_stats_28, ANN_metrics]

metrics_df = pd.DataFrame(data=metrics, index=['Cement (Ignoring Cure␣
↪Time)','Cementitious_Ratio (Ignoring Cure Time)','Fly_Ash_Ratio (Ignoring␣
↪Cure Time)','Superplasticizer_Ratio (Ignoring Cure Time)','ANN (Function of␣
↪Time)'], columns=['MAE','MSE','RMSE'])
metrics_28_df = pd.DataFrame(data=metrics_28, index=['Cement (Cure Time = 28␣
↪Days)','Cementitious_Ratio (Cure Time = 28 Days)','Fly_Ash_Ratio (Cure Time␣
↪= 28 Days)','Superplasticizer_Ratio (Cure Time = 28 Days)','ANN (Function of␣
↪Time)'], columns=['MAE','MSE','RMSE'])
```

[104]:
```
metrics_df
```

[104]:

	MAE	MSE	RMSE
Cement (Ignoring Cure Time)	11.555613	192.784799	13.884697
Cementitious_Ratio (Ignoring Cure Time)	12.834673	253.058148	15.907801
Fly_Ash_Ratio (Ignoring Cure Time)	12.121987	212.894325	14.590899
Superplasticizer_Ratio (Ignoring Cure Time)	12.189767	225.909298	15.030279
ANN (Function of Time)	5.083552	41.815519	6.466492

[105]:
```
metrics_28_df
```

[105]:

	MAE	MSE	RMSE
Cement (Cure Time = 28 Days)	9.134082	140.117503	11.837124
Cementitious_Ratio (Cure Time = 28 Days)	11.519580	197.957201	14.069726
Fly_Ash_Ratio (Cure Time = 28 Days)	7.692695	91.317960	9.556043
Superplasticizer_Ratio (Cure Time = 28 Days)	11.954354	243.970379	15.619551
ANN (Function of Time)	5.083552	41.815519	6.466492

1.13 Conclusions & Recommendations

By comparing the evaluation metrics for all models, we conclude that the ANN model performed significantly better than all of the linear models. It outperformed the best linear model's RMSE (for Fly_Ash_Ratio at 28 Days) by over 30%! An important note is that the linear models were not scaled, and the ANN model was. We kept the linear models biased in order to maintain coefficient interpretabililty, whereas that was not relevant to the ANN model.

What is surprising is that the ANN model still outperformed the linear models, even when controlling for cure time at 28 days. Perhaps the most startling insight is that the fly ash ratio was even more accurate at predicting concrete compressive strength than the cement quantity, to the point that it had the lowest errors of all of the linear models. We therefore recommend that engineers give very conservative fly ash ratio specifications when allowing substitutions for Portland cement.