hw1

October 18, 2023

[ ]:
```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
import sklearn.model_selection
import sklearn.preprocessing
```

0.1 Preprocessing Work

[ ]:
```
data = pd.read_excel("Concrete_Data.xls")
shortenedCols = ["Cement", "Slag", "Ash", "Water", "Superplasticizer",␣
 ↪"Coarse", "Fine", "Age", "Strength"]
newCols = dict(zip(data.columns, shortenedCols))

renamed = data.rename(columns=newCols)
data.head()
```

[ ]:
```
   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
```

[ ]:

```
train_size = 900/renamed.shape[0]
assert(train_size == 900/1030)

y = renamed["Strength"]
X = renamed.drop(columns="Strength")

X_train, X_test, y_train, y_test = sklearn.model_selection.train_test_split(X,
 ↪y, train_size=train_size)
X_train = np.array(X_train)
X_test = np.array(X_test)
y_train = np.array(y_train)
y_test = np.array(y_test)
```

[ ]:
```
scaler = sklearn.preprocessing.StandardScaler()
X_scaler = scaler.fit(X_train)

X_train_norm = np.array(X_scaler.transform(X_train))
X_test_norm = np.array(X_scaler.transform(X_test))

y_scaler = sklearn.preprocessing.StandardScaler()
y_scaler.fit(y_train.reshape(-1, 1))
y_train_norm = y_scaler.transform(y_train.reshape(-1, 1)).ravel()
y_test_norm = y_scaler.transform(y_test.reshape(-1, 1)).ravel()
```

[ ]:
```
# This function was used to generate the plots in the report
# I have disabled its execution to save space in the final report

def feature_dist(df):
    for feature in shortenedCols:
        plt.figure(figsize=(3, 2))
        plt.hist(df[feature], bins=50)
        plt.title(f'Distribution of {feature}')
        plt.xlabel(feature)
        plt.ylabel('Frequency')
        plt.show()

# feature_dist(renamed)
```

0.2 Gradient Descent Algorithm

[ ]:
```
def gradient_descent(X, y, learning_rate, iterations):
    X = np.c_[np.ones(X.shape[0]), X]
    theta = np.zeros(X.shape[1])
    for _ in range(iterations):
        error = np.dot(X, theta.T) - y
        gradient = (2 / len(y)) * np.dot(X.T, error)
        theta = theta - (learning_rate * gradient)

    return theta
```

0.2.1 Univariate Model

For each feature, we calculate the unnormalized and normalized theta values. Before running the gradient descent algorithm, we concatenate a column of 1s before our feature to account for the “constant” offset term. Therefore, we get two theta values back per run. The first corresponds to the constant, and the second corresponds to the scale of the first feature.

It’s important to note the difference in learning rate between the unnormalized and normalized values. Because of the larger unnormalzied values, running the algorithm with a larger learning rate will cause our numbers to overflow. This is partially accounted for by increasing the number of iterations.

[ ]:
```
thetas = np.zeros([8,2])
norm_thetas = np.zeros([8, 2])
for i in range(8):
    target = np.array(X_train[:, i]).reshape(-1,1)
    thetas[i] = gradient_descent(target, y_train, 0.000001, 1000)

    norm_target = np.array(X_train_norm[:, i]).reshape(-1,1)
    norm_thetas[i] = gradient_descent(norm_target, y_train_norm, 0.005, 10000)

print(thetas)
print(norm_thetas)
```

```
[[0.0034637  0.12030553]
 [0.03997999 0.21899004]
 [0.04575242 0.25362762]
 [0.00310929 0.19011898]
 [0.06798608 0.47597249]
 [0.00096533 0.03601923]
 [0.00141427 0.04509721]
 [0.04412275 0.3226835 ]]
[[ 5.55308885e-17  5.02343218e-01]
 [ 1.38733469e-16  1.46692528e-01]
 [ 1.28356585e-16 -1.12944599e-01]
 [-3.46991571e-16 -2.87010654e-01]
 [ 1.52643330e-16  3.66130334e-01]
 [ 2.86180955e-16 -1.71369193e-01]
 [ 2.49810049e-16 -1.75216548e-01]
 [ 1.21386851e-16  3.30158472e-01]]
```

0.3 Multivariate Model

This uses the exact same function defined above, yet the entire input is passed to the gradient descent algorithm instead of just a single feature. We expect the output of each function to be a 1x9 array, accounting for the extra constant column of 1s.

[ ]:
```
multivar_thetas = gradient_descent(X_train, y_train, 0.0000001, 10000)
multivar_norm_thetas = gradient_descent(X_train_norm, y_train_norm, 0.01, 1000)

print(multivar_thetas)
print(multivar_norm_thetas)
```

```
[-4.94565987e-05  1.17061494e-01  9.58321104e-02  8.95407190e-02
 -1.34837471e-01  3.34834230e-02  7.90934998e-04  1.21552682e-02
  1.04428152e-01]
[-3.87443164e-16  5.73305067e-01  3.59729574e-01  1.79375515e-01
 -3.32187173e-01  8.88597157e-02 -5.12532722e-02 -7.57791740e-02
  4.21943592e-01]
```

0.4 Training Model Performance

[ ]:
```python
def predict(X, thetas):
    preds = np.dot(X, thetas.T)
    return preds

def mse(y, y_pred):
    return np.sum(np.square(y - y_pred)) / np.size(y)
```

[ ]:
```python
print("Performance on Training Dataset")
print("RSquared\t\t MSE\t\t Variance")

X_multivar_train = np.c_[np.ones(X_train.shape[0]), X_train]
y_pred = predict(X_multivar_train, multivar_thetas)
MSE = mse(y_train, y_pred)
var = np.var(y_train)
rsquared = 1 - (MSE/var)
print(f"{rsquared}, {MSE}, {var} = Unnormalized Multivariate R^2")

X_multivar_norm_train = np.c_[np.ones(X_train_norm.shape[0]), X_train_norm]
y_pred = predict(X_multivar_norm_train, multivar_norm_thetas)
MSE = mse(y_train_norm, y_pred)
var = np.var(y_train_norm)
rsquared = 1 - (MSE/var)
print(f"{rsquared}, {MSE}, {var} = Normalized Multivariate R^2\n")


for i in range(8):
    target = np.c_[np.ones((X_train.shape[0], 1)), X_train[:,i]]
    y_pred = predict(target, thetas[i])
    MSE = mse(y_train, y_pred)
    var = np.var(y_train)
    rsquared = 1 - (MSE/var)
    print(f"{rsquared}, {MSE}, {var} = R^2 for Unnormalized Feature␣
 ↪{shortenedCols[i]}")

print("")

for i in range(8):
    target = np.c_[np.ones((X_train_norm.shape[0], 1)), X_train_norm[:,i]]
    y_pred = predict(target, norm_thetas[i])
    MSE = mse(y_train_norm, y_pred)
    var = np.var(y_train_norm)
    rsquared = 1 - (MSE/var)
    print(f"{rsquared}, {MSE}, {var} = R^2 for Normalized Feature␣
 ↪{shortenedCols[i]}")
```

```
Performance on Training Dataset
```

```
RSquared                 MSE             Variance
0.6056716878185033, 110.91766254069823, 281.28252299988645 = Unnormalized
Multivariate R^2
0.6143422909001132, 0.38565770909988684, 1.0 = Normalized Multivariate R^2

0.18211356369270126, 230.05716033190294, 281.28252299988645 = R^2 for
Unnormalized Feature Cement
-2.2763111974318657, 921.5690797464143, 281.28252299988645 = R^2 for
Unnormalized Feature Slag
-2.87211977997769, 1089.15962106989, 281.28252299988645 = R^2 for Unnormalized
Feature Ash
-0.20024187017790296, 337.60706145374274, 281.28252299988645 = R^2 for
Unnormalized Feature Water
-3.664915222607407, 1312.1591233955883, 281.28252299988645 = R^2 for
Unnormalized Feature Superplasticizer
-0.08772754903166602, 305.9587493281097, 281.28252299988645 = R^2 for
Unnormalized Feature Coarse
-0.12338612287634709, 315.98888294571935, 281.28252299988645 = R^2 for
Unnormalized Feature Fine
-2.2268732003673697, 907.6630352000519, 281.28252299988645 = R^2 for
Unnormalized Feature Age

0.25234870854805735, 0.7476512914519426, 1.0 = R^2 for Normalized Feature Cement
0.021518697850317757, 0.9784813021496824, 1.0 = R^2 for Normalized Feature Slag
0.012756482449876483, 0.9872435175501235, 1.0 = R^2 for Normalized Feature Ash
0.08237511534942799, 0.917624884650572, 1.0 = R^2 for Normalized Feature Water
0.13405142172356965, 0.8659485782764303, 1.0 = R^2 for Normalized Feature
Superplasticizer
0.029367400160310808, 0.9706325998396892, 1.0 = R^2 for Normalized Feature
Coarse
0.030700838713056733, 0.9692991612869433, 1.0 = R^2 for Normalized Feature Fine
0.10900461661907535, 0.8909953833809247, 1.0 = R^2 for Normalized Feature Age
```

0.5 Testing Model Performance

[ ]:
```python
print("Performance on Testing Dataset")
print("RSquared\t\t MSE\t\t Variance")

X_multivar_test = np.c_[np.ones(X_test.shape[0]), X_test]
y_pred = predict(X_multivar_test, multivar_thetas)
MSE = mse(y_test, y_pred)
var = np.var(y_test)
rsquared = 1 - (MSE/var)
print(f"{rsquared}, {MSE}, {var} = Unnormalized Multivariate R^2")

X_multivar_norm_test = np.c_[np.ones((X_test_norm.shape[0], 1)), X_test_norm]
y_pred = predict(X_multivar_norm_test, multivar_norm_thetas)
```

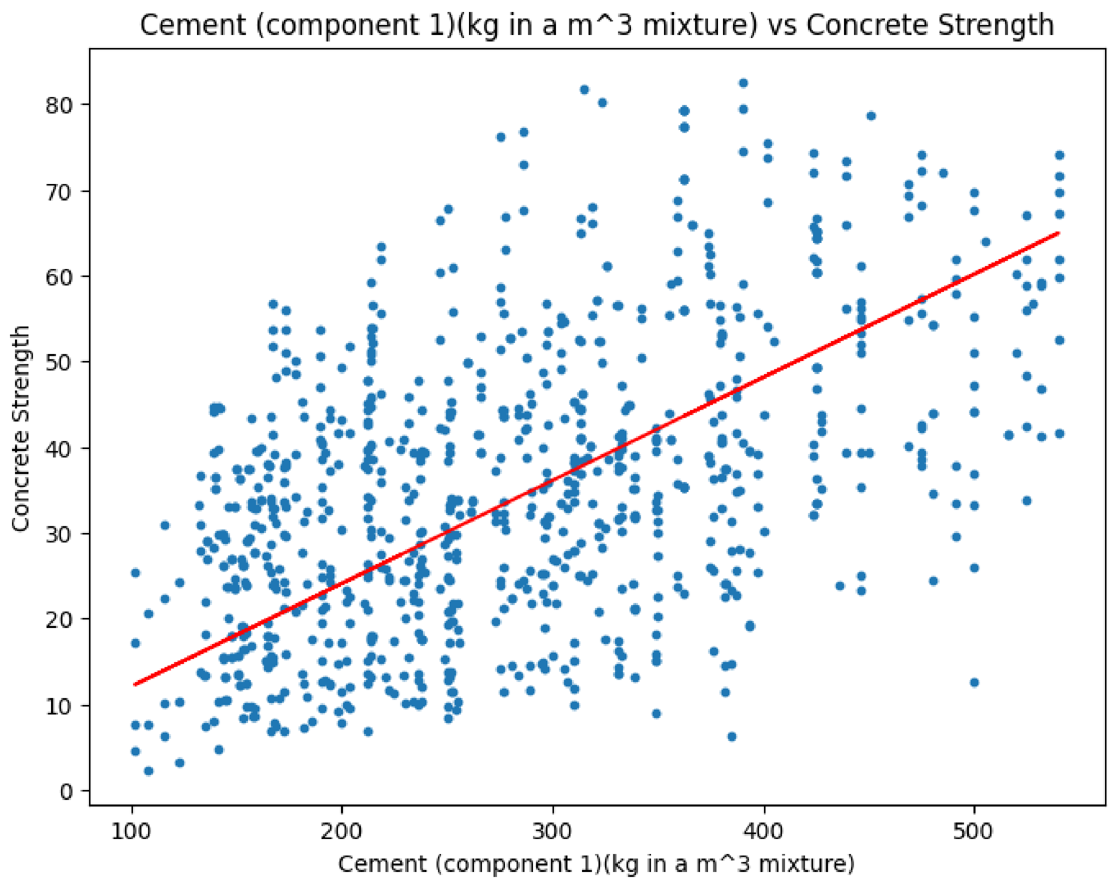
```
MSE = mse(y_test_norm, y_pred)
var = np.var(y_test_norm)
rsquared = 1 - (MSE/var)
print(f"{rsquared}, {MSE}, {var} = Normalized Multivariate R^2\n")


for i in range(8):
    target = np.c_[np.ones((X_test.shape[0], 1)), X_test[:,i]]
    y_pred = predict(target, thetas[i])
    MSE = mse(y_test, y_pred)
    var = np.var(y_test)
    rsquared = 1 - (MSE/var)
    print(f"{rsquared}, {MSE}, {var} = R^2 for Unnormalized Feature␣
 ↪{shortenedCols[i]}")

print("")

for i in range(8):
    target = np.c_[np.ones((X_test_norm.shape[0], 1)), X_test_norm[:,i]]
    y_pred = predict(target, norm_thetas[i])
    MSE = mse(y_test_norm, y_pred)
    var = np.var(y_test_norm)
    rsquared = 1 - (MSE/var)
    print(f"{rsquared}, {MSE}, {var} = R^2 for Normalized Feature␣
 ↪{shortenedCols[i]}")
```

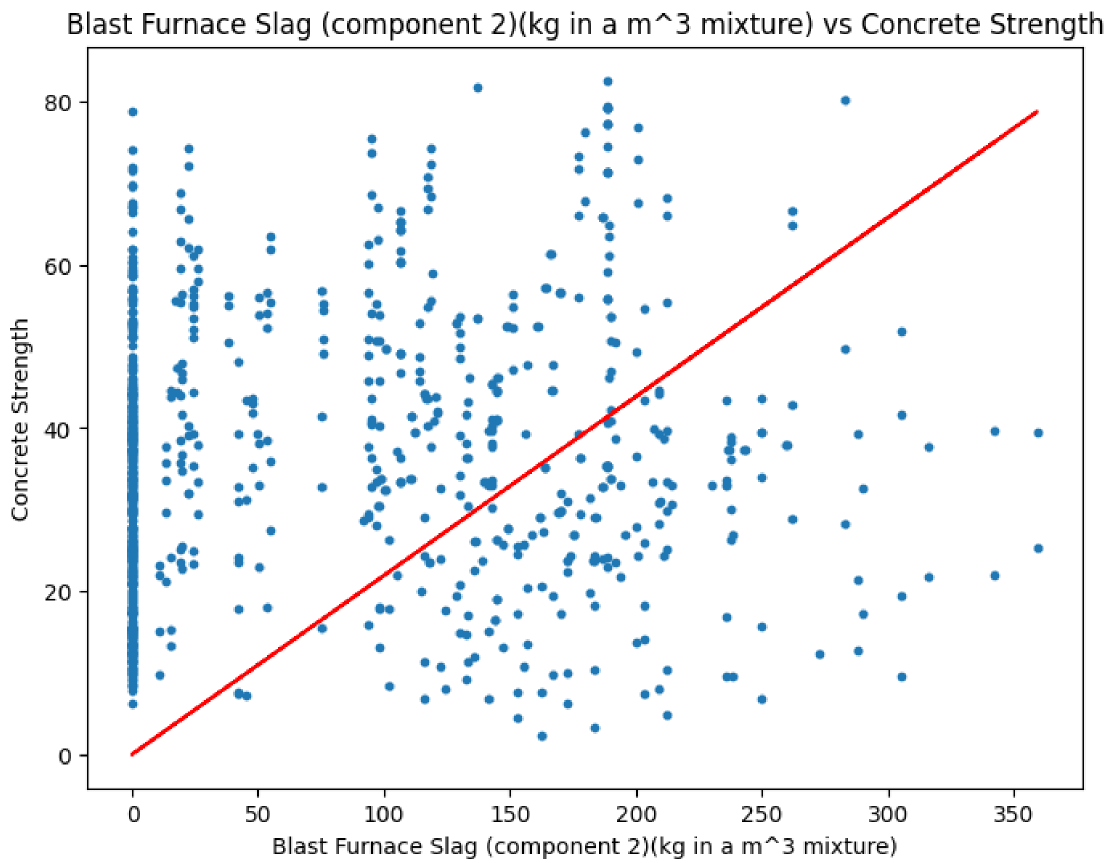
```
Performance on Testing Dataset
RSquared                 MSE               Variance
0.5537961158499328, 114.75321894547034, 257.1766473168498 = Unnormalized
Multivariate R^2
0.5717923301901839, 0.39151032813045994, 0.9143001298980588 = Normalized
Multivariate R^2

0.05295064793759763, 243.5589772070036, 257.1766473168498 = R^2 for Unnormalized
Feature Cement
-2.9789647029597193, 1023.2968020992658, 257.1766473168498 = R^2 for
Unnormalized Feature Slag
-3.0935869602781816, 1052.7749699443173, 257.1766473168498 = R^2 for
Unnormalized Feature Ash
-0.26953186303719656, 326.4939481978204, 257.1766473168498 = R^2 for
Unnormalized Feature Water
-4.584213974528381, 1436.1294278691096, 257.1766473168498 = R^2 for Unnormalized
Feature Superplasticizer
-0.08806069419969553, 279.82380141152186, 257.1766473168498 = R^2 for
Unnormalized Feature Coarse
-0.1341197658079767, 291.66911902626634, 257.1766473168498 = R^2 for
Unnormalized Feature Fine
```

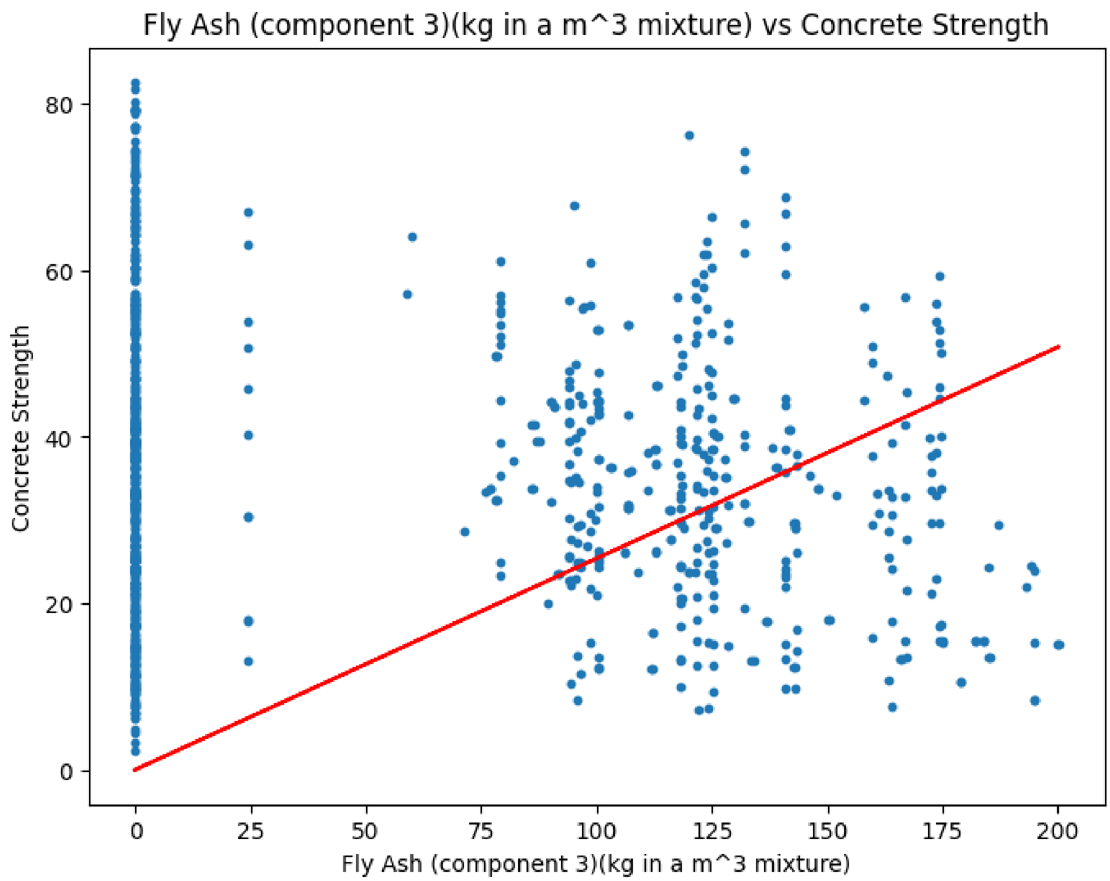
```
-2.6874385052329544, 948.3230719628674, 257.1766473168498 = R^2 for Unnormalized
Feature Age

0.19548643481707606, 0.7355668571514977, 0.9143001298980588 = R^2 for Normalized
Feature Cement
-0.027999295268484214, 0.9398998891990881, 0.9143001298980588 = R^2 for
Normalized Feature Slag
-0.021315368261298984, 0.9337887738681894, 0.9143001298980588 = R^2 for
Normalized Feature Ash
0.07601524974208251, 0.8447993771846394, 0.9143001298980588 = R^2 for Normalized
Feature Water
0.1165907335861569, 0.8077012070353256, 0.9143001298980588 = R^2 for Normalized
Feature Superplasticizer
-0.008560540991194188, 0.9221270336383053, 0.9143001298980588 = R^2 for
Normalized Feature Coarse
-0.01346193263703599, 0.9266083766567798, 0.9143001298980588 = R^2 for
Normalized Feature Fine
0.08400049819338729, 0.8374984634883431, 0.9143001298980588 = R^2 for Normalized
Feature Age
```

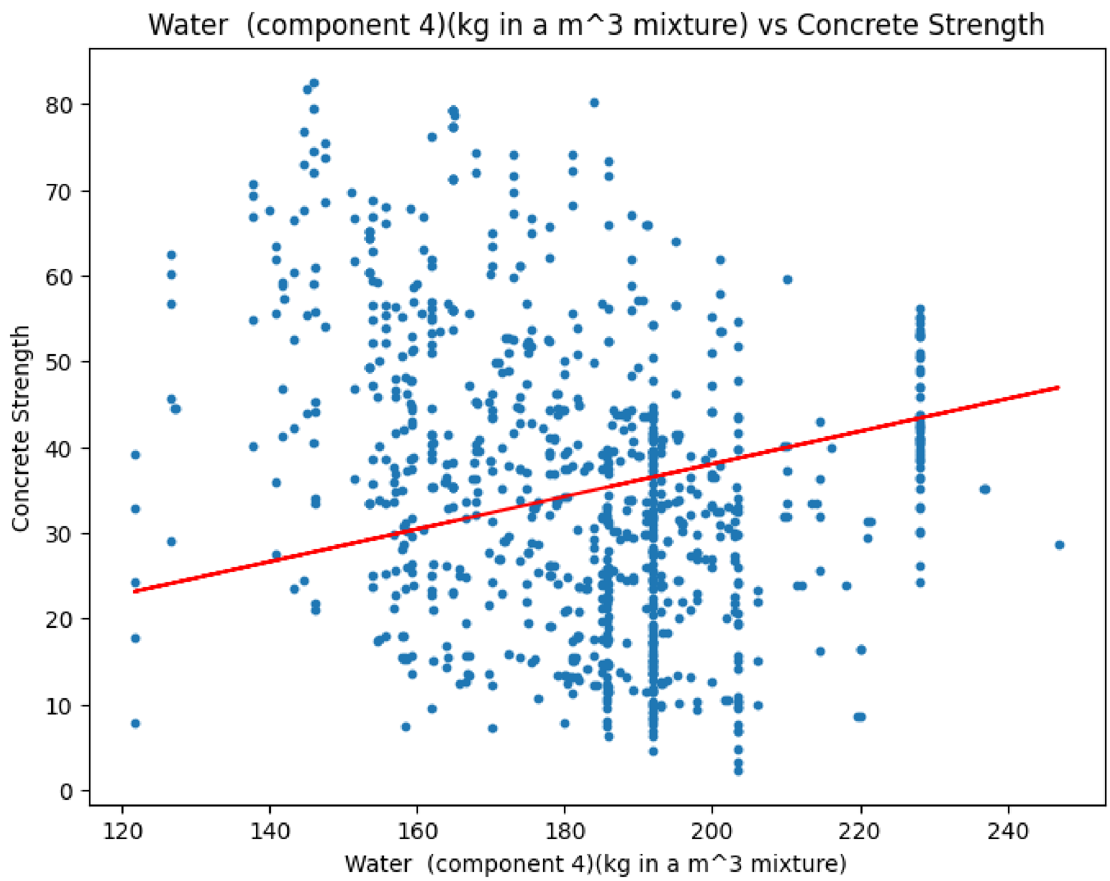
[ ]:

```python
# Plots of your univariate models on top of scatterplots of the training data
# used. Please plot the data using the x-axis for the predictor variable and␣
↪the y-axis
# for the response variable.

for i in range(8):
    target = np.array(X_train[:, i])
    plt.figure(figsize=(8, 6))
    plt.scatter(target, y_train, s=10)
    plt.plot(target, np.dot(np.c_[np.ones(target.shape), target], thetas[i].T),␣
↪color='r')
    plt.xlabel(data.columns[i])
    plt.ylabel('Concrete Strength')
    plt.title(data.columns[i] + " vs Concrete Strength")
    plt.show()
```

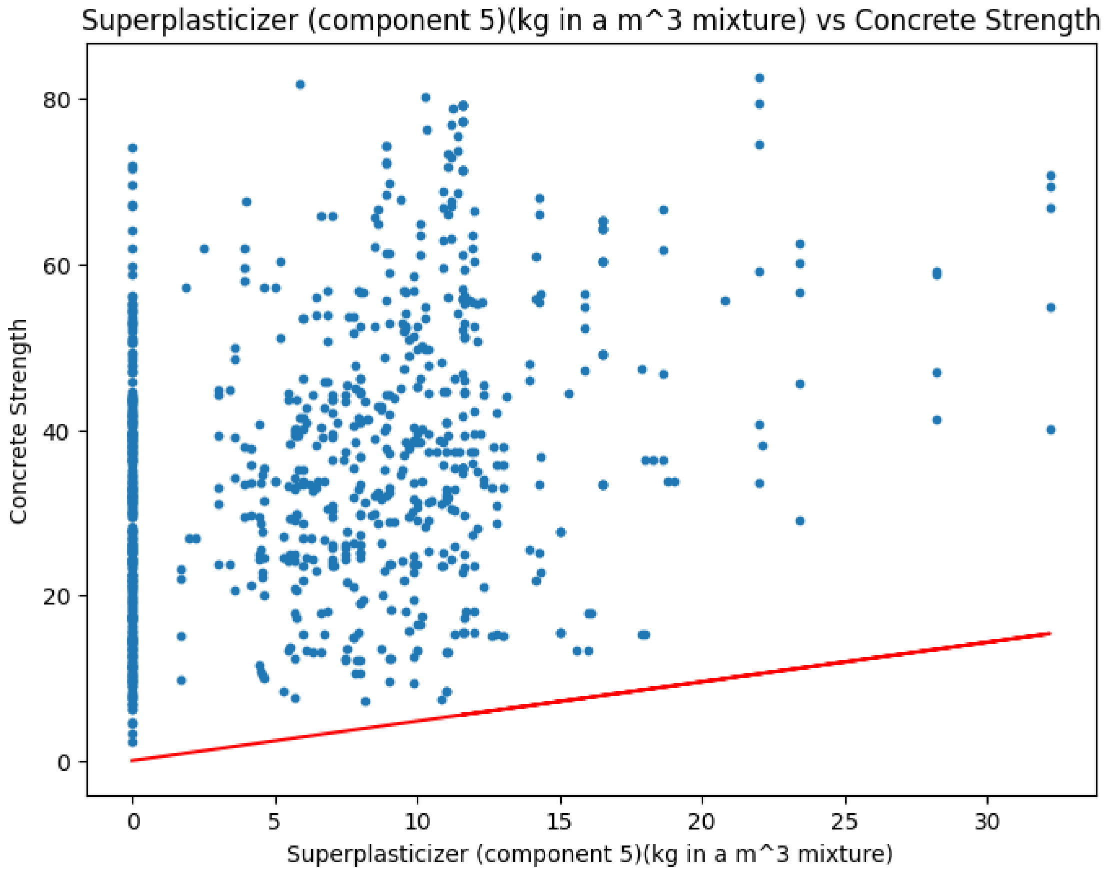

Cement (component 1)(kg in a m^3 mixture) vs Concrete Strength
Concrete Strength
Cement (component 1)(kg in a m^3 mixture)
0
10
20
30
40
50
60
70
80
100
200
300
400
500

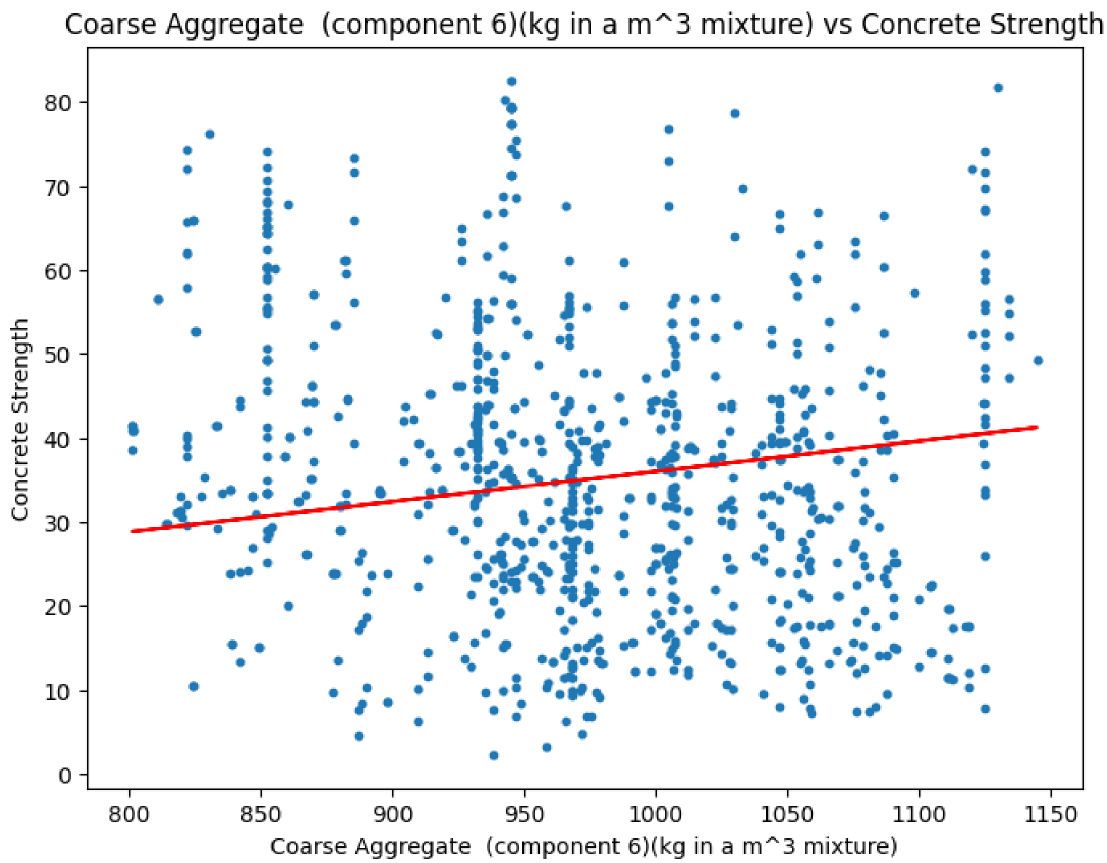

Blast Furnace Slag (component 2)(kg in a m^3 mixture) vs Concrete Strength
Concrete Strength
0
20
40
60
80
0
50
100
150
200
250
300
350
Blast Furnace Slag (component 2)(kg in a m^3 mixture)

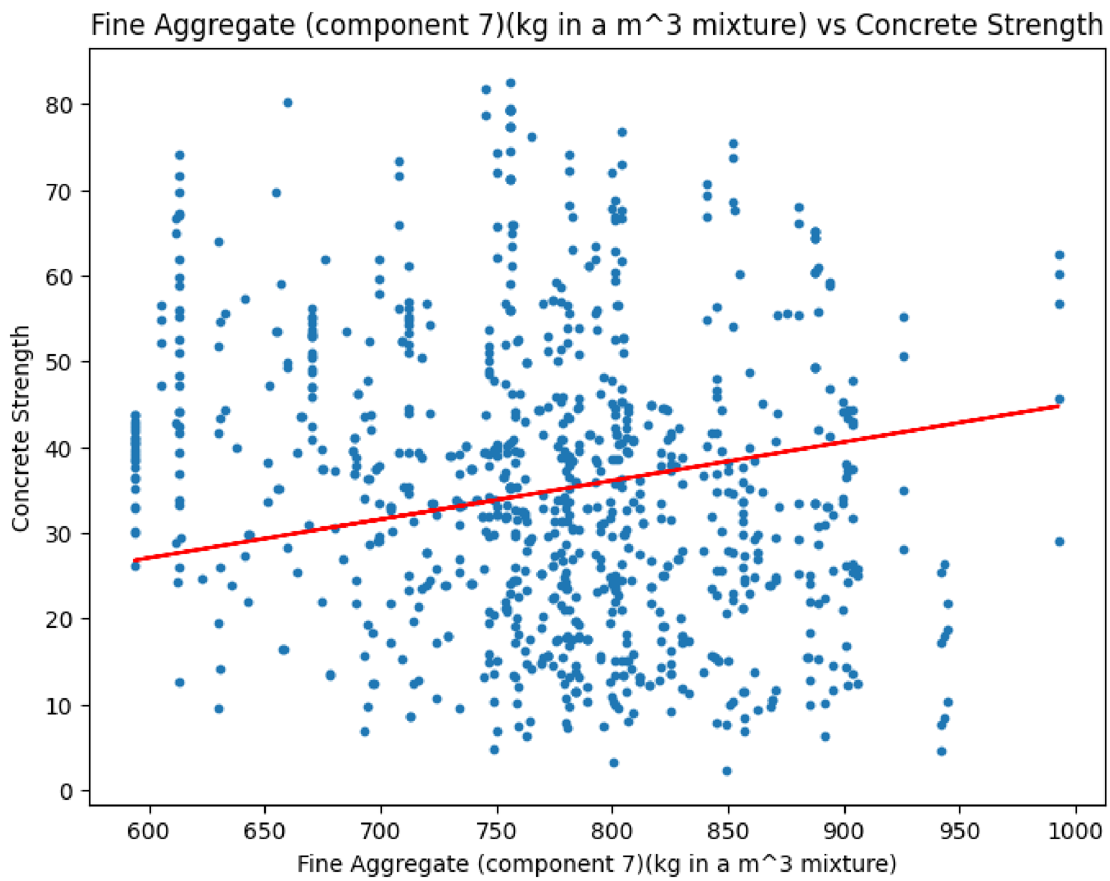

Fly Ash (component 3)(kg in a m^3 mixture) vs Concrete Strength
Concrete Strength
0
20
40
60
80
0
25
50
75
100
125
150
175
200
Fly Ash (component 3)(kg in a m^3 mixture)

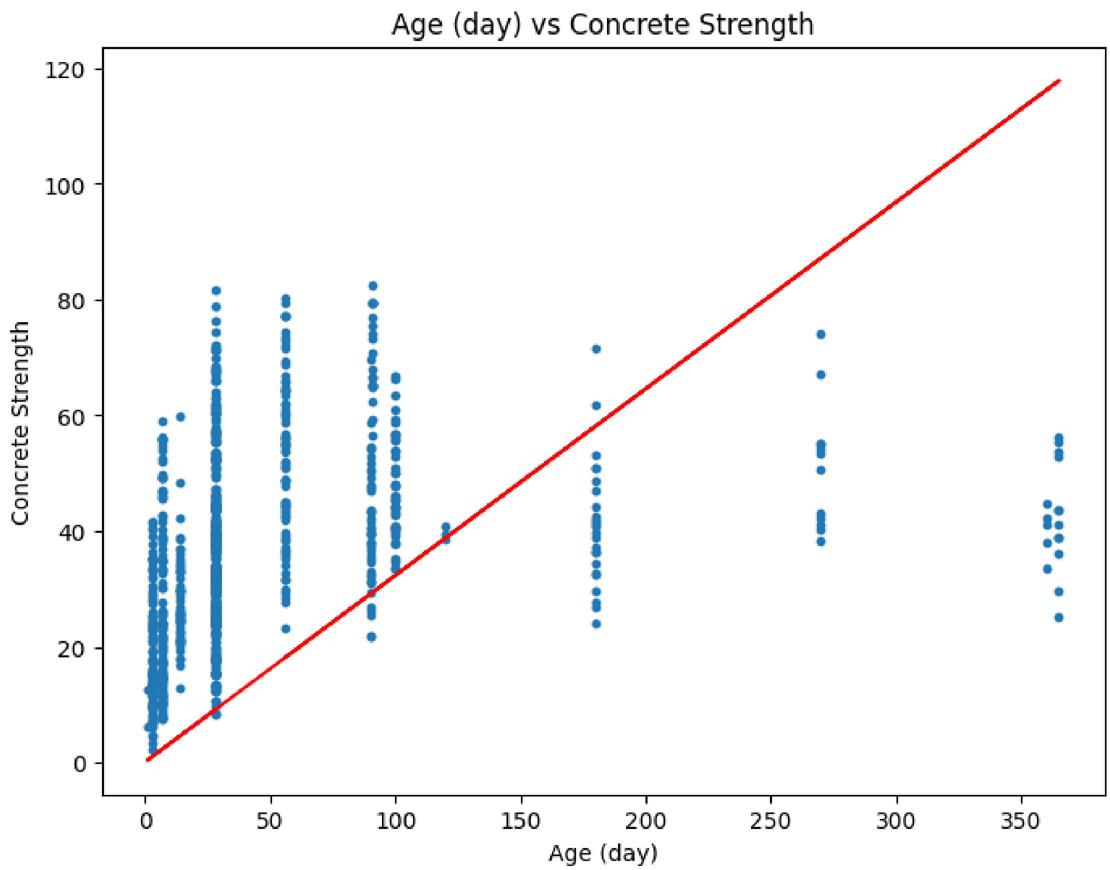


Water (component 4)(kg in a m^3 mixture) vs Concrete Strength
Concrete Strength
Water (component 4)(kg in a m^3 mixture)
0
10
20
30
40
50
60
70
80
120
140
160
180
200
220
240


Superplasticizer (component 5)(kg in a m^3 mixture) vs Concrete Strength
Concrete Strength
Superplasticizer (component 5)(kg in a m^3 mixture)
0
20
40
60
80
0
5
10
15
20
25
30


Coarse Aggregate (component 6)(kg in a m^3 mixture) vs Concrete Strength
Concrete Strength
Coarse Aggregate (component 6)(kg in a m^3 mixture)
0
10
20
30
40
50
60
70
80
800
850
900
950
1000
1050
1100
1150


Fine Aggregate (component 7)(kg in a m^3 mixture) vs Concrete Strength
Concrete Strength
0
10
20
30
40
50
60
70
80
600
650
700
750
800
850
900
950
1000
Fine Aggregate (component 7)(kg in a m^3 mixture)


Age (day) vs Concrete Strength
Concrete Strength
Age (day)
0
20
40
60
80
100
120
0
50
100
150
200
250
300
350