CSE 514 – Spring 2022 Programming Assignment 1

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1.Introduction

1.1 The description of the problem

Given a dataset of Concrete Compressive Strength in the UCI repository, we need to design and implement a (stochastic) gradient descent algorithm or algorithms for regression to calculate "the capacity of concrete to withstand loads before failure"[1] after considered eight features: Cement, Blast Furnace Slag, Fly Ash, Water, Superplasticizer, Coarse Aggregate, Fine Aggregate and Age(day). I will utilize Python and it's related fundamental package, such as Numpy, Pandas and Matplotlib, to solve following questions in a Jupyter Notebook file. Please check the file named '**ReadMe**' to run codes. Here is my general answer description for each question:

a) For question A, I will apply the gradient descent algorithm for optimizing a uni-variate linear regression model of eight characters as above.
b) For question B, the variation of the regression model should be all of the features plusing one(b). Both question will utilize MSE(mean squared error) as the loss function.
c) For the question C, what I should extended is a multi-variate quadratic regression model, which has 36 quadratic terms, such as: $x_1^2,\cdots,x_8^2,x_1x_2,\cdots,x_7x_8$, and eight linear terms. The apply multi-variate regression model to calculate and evaluate.
d) For the question D, I will try to normalize or standardize each variable, as some characters, such like Age and Cement, do not have same unit of measurement.

1.2 Details of algorithm

Generally speaking, the stopping criterion would be complete the total times of passes of the entire training dataset that I initialed before start, for example, if I assume the "epoch" is 500, it means that the model will stop as long as it has finished 500 times. Besides, for this gradient descent model, I will initial a pivot learning rate at first, and find the most suitable one after trail and error!

For each question, the steps and relevant formulas is as followed:
A) Uni-variate linear regression
The model formula should be:

$$f(x) = mx + b$$

Lose function(here I used MSE) should be:

$$L(m,b) = \frac{1}{n}\sum_{i=1}^{n}(y_i - (mx_i + b))^2$$

Since I need to optimize this uni-variate linear regression model, the partical derivative of the loss function should be calcuate, and update the coefficient m and n for eight variables. Besides, I assume that α is the learning rate, and it could be initilized as $\alpha = 1\times 10^{-11}$ the eqution should be:

$$\begin{cases} \frac{\partial L}{\partial m} = \frac{1}{n}\sum_{i=1}^{n}(-2x_i(y_i - (mx_i + b))) \\ \frac{\partial L}{\partial b} = \frac{1}{n}\sum_{i=1}^{n}(-2(y_i - (mx_i + b))) \end{cases}$$

Therefore, for each step, the updating formula of m and b should be:

$$\begin{cases} m_{new} = m_{old} - \frac{\alpha}{n}\sum_{i=1}^{n}(-2x_i(y_i - (m_{old}x_i + b_{old}))) \\ b_{old} = b_{old} - \frac{\alpha}{n}\sum_{i=1}^{n}(-2(y_i - (m_{old}x_i + b_{old}))) \end{cases}$$

The stopping criterion should be(I assumed): 500

B)Multi-variate linear regression
The high level idea of solving multi-variate linear regression is slightly different with uni-variate linear regression. For this problem, it needs to consider more than one variate's influence for the concrete compressive strength. Given conditions above, the formula of this problem should be:

$$\begin{cases} y = f(x) = (\vec{m}\cdot \vec{x}) = m_0x_0 + m_1x_1 + m_2x_2 + \cdots + m_8x_8 \\ \vec{m} = (m_0, m_1, m_1, \cdots, m_8)^T \\ \vec{x} = (x_0, x_1, x_1, \cdots, x_8)^T \\ x_0 = 1 \end{cases}$$

Meanwhile, the loss function should be:

$$L(m) = \frac{1}{n}\sum_{i=1}^{n}(y_{predicted} - y_i)^2 = \frac{1}{n}((m_0x_0 + m_1x_1 + \ldots + m_8x_8) - y_i)^2$$

The updating formula of m should be:

$$\vec{m}_{new} = \vec{m}_{old} - \alpha \cdot \frac{\partial L}{\partial \vec{m}} = \vec{m}_{old} - \alpha \cdot (2/n)(\vec{x})(\vec{a}\cdot \vec{x} - \vec{y})$$

The order of y_predicted and y_i should be noticed, as it decides whether we need add minus sign during seeking for derivation or not.

1.3 Pseudo-code of algorithms

For the **Question A**, the pseudo-code should be as followed:

```
//Initialization
Int n is assumed iteration times(epoches)
Int m = b = 0
Int $\alpha$ is learning rate, and could be initilized as $\alpha = 1e-6$
Int $x_i, y_i$ is traing variable input and training variable out put

● Function uni_variate_linear_regression_model_training
  (current_character_m_b, x_training ,y_training, lr, epoches):
    Record the size of x_training as n
    $f(x) = mx + b$
    $m = m - \frac{-2\alpha}{n}\sum_{i=1}^{n}(x_i(y_i - (mx_i + b)))$
    $b = b - \frac{-2\alpha}{n}\sum_{i=1}^{n}((y_i - (mx_i + b)))$

    Print the current feature variable
    Return coefficient m and b
```

```
● Function uni_variate_linear_regression_model(x_training,
  y_training,x_testing, y_testing, current_character_m_b):
    Record the size of x_training and x_testing separetly
    Calculate MSE for training and testing set by using:
    $MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - (mx_i + b))^{2}$
    Print out the result
    Return

● Function calculate_current_character_variance(y):
    Calculate variance by utilizing sum, mean and square value
● Function calculate_current_character_variance_explained
  (current_character_variance, final_model_trained_mse)
    Result shoud be  1 - (final_model_trained_mse[0] /
    current_character_variance)
```

Call function uni_variate_linear_regression_model_training to calculate coefficient m and b, and the second function is to calculate MSE value. Then use rest of function to get variance explained for the response variable.

Draw the plot for later use.

For the **Question B**, the pseudo-code should be as followed:
Add a column of ones before the head of training and testing set
Initial a learning rate lr = 5.8e-7 and epoches should be 500

```
● Function multi_variate_linear_regression_training (x_training,
  y_training, lr, epoches):
    Initialize $m = [0,0,0,...,0]$
    Int n is assumed iteration times
    While  interationTimes <=n  {

      $m = m - lr \cdot (2/n)(\vec{x})(\vec{m} \cdot \vec{x} - \vec{y})$
    Return m
    }
```

- Function multi_variate_linear_regression_model (current_character_m, x_training, y_training, x_testing, y_testing):

  Calculate MSE $m = (1/2)\cdot(\vec{x}\cdot\vec{m} - y)^2$

Calculate the variance explained of multi-variate regression model for all characters

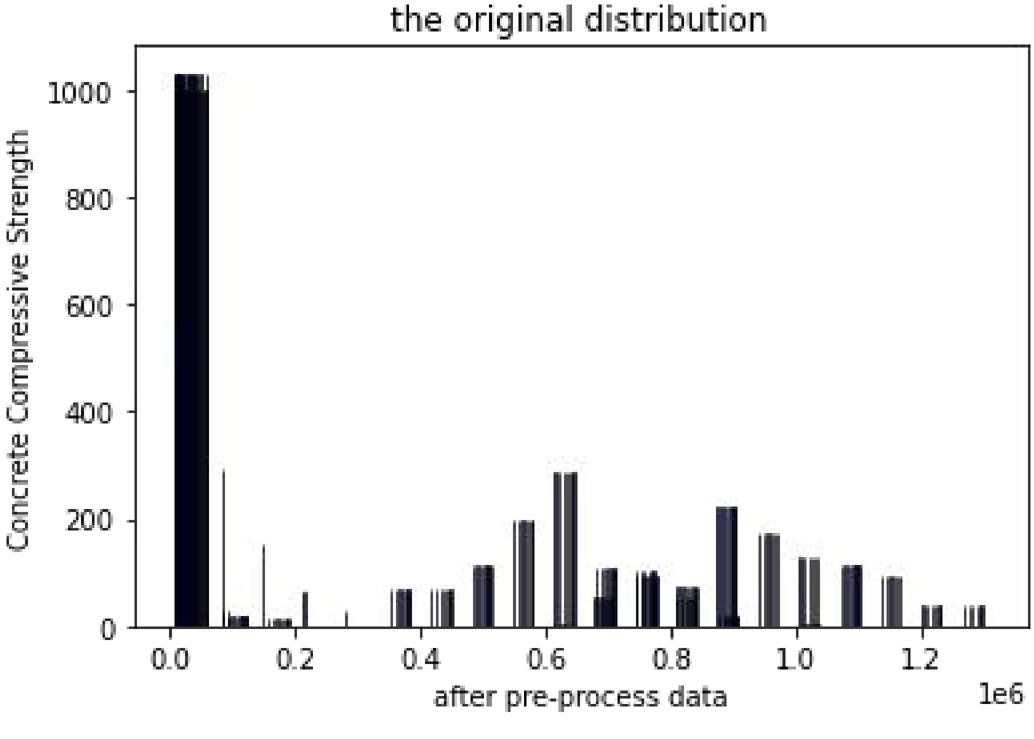
For the **Question C,** what I should extended is a multi-variate quadratic regression model, which has 36 quadratic terms, and eight linear terms.

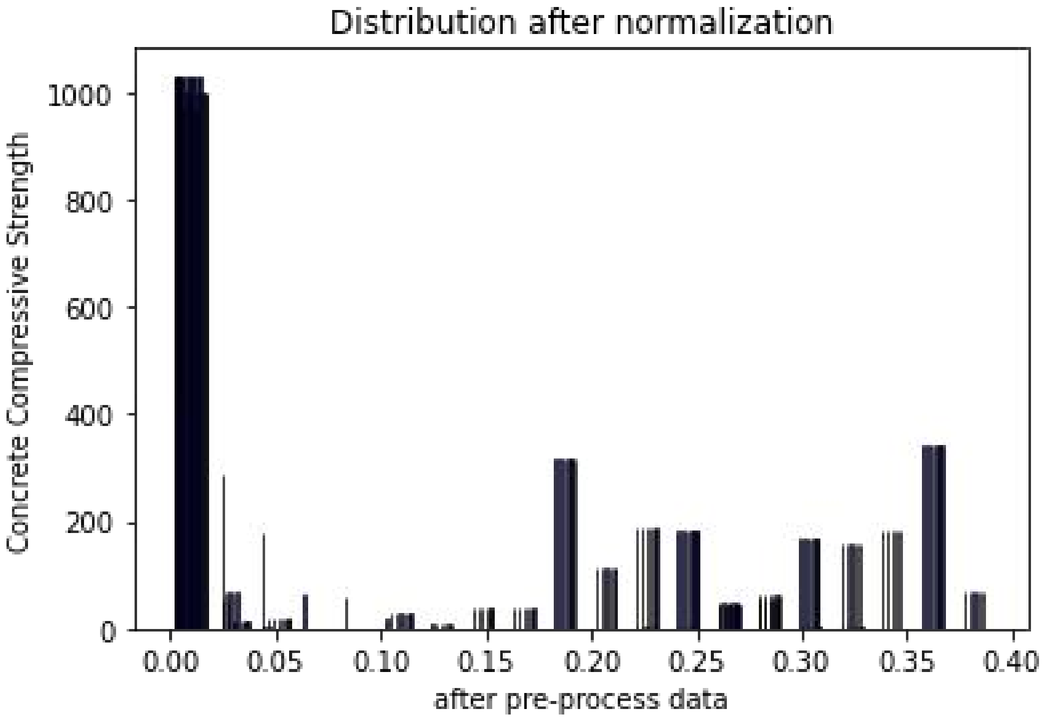
- Function reshape_a_new_dataset(data):

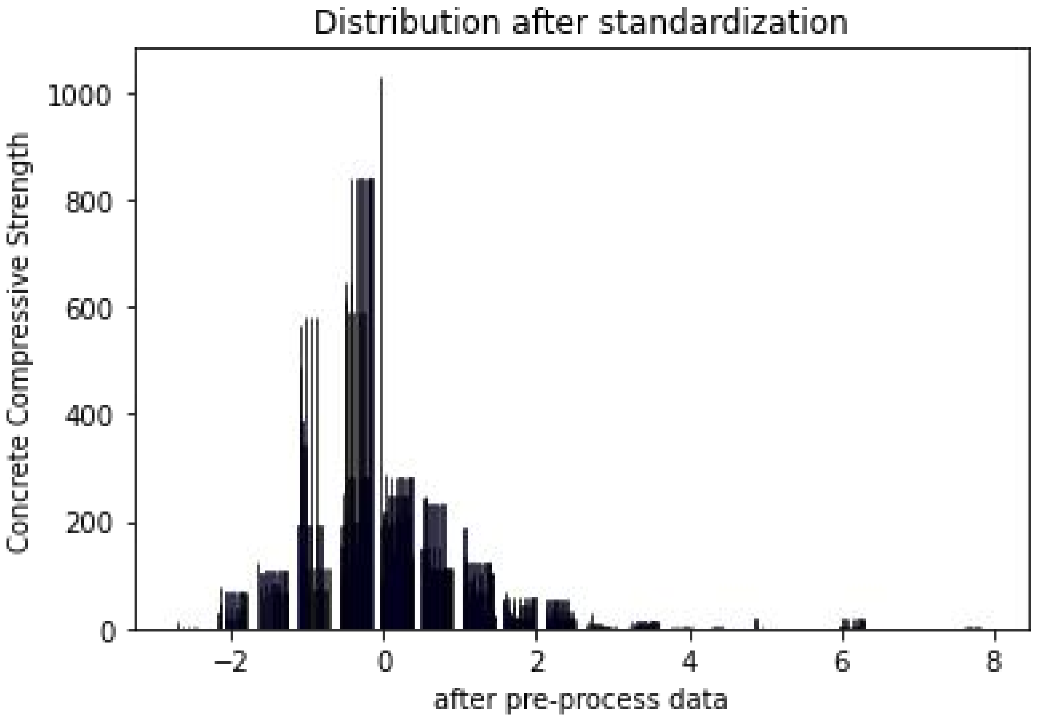
  Initial i, j for two while loop to calculate x1^2, x1 * x2, ..., x8^2

  And use the model just like Question B to get the result

For the **Question D**, I will try to normalize or standardize each variable, as some variables, such like Age and Cement, do not have the same unit of measurement. I imported StandardScaler, Normalizer from sklearn.preprocessing to process data.




Distribution after normalization
Concrete Compressive Strength
0
200
400
600
800
1000
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
after pre-process data


Distribution after standardization
Concrete Compressive Strength
0
200
400
600
800
1000
−2
0
2
4
6
8
after pre-process data

2.Result

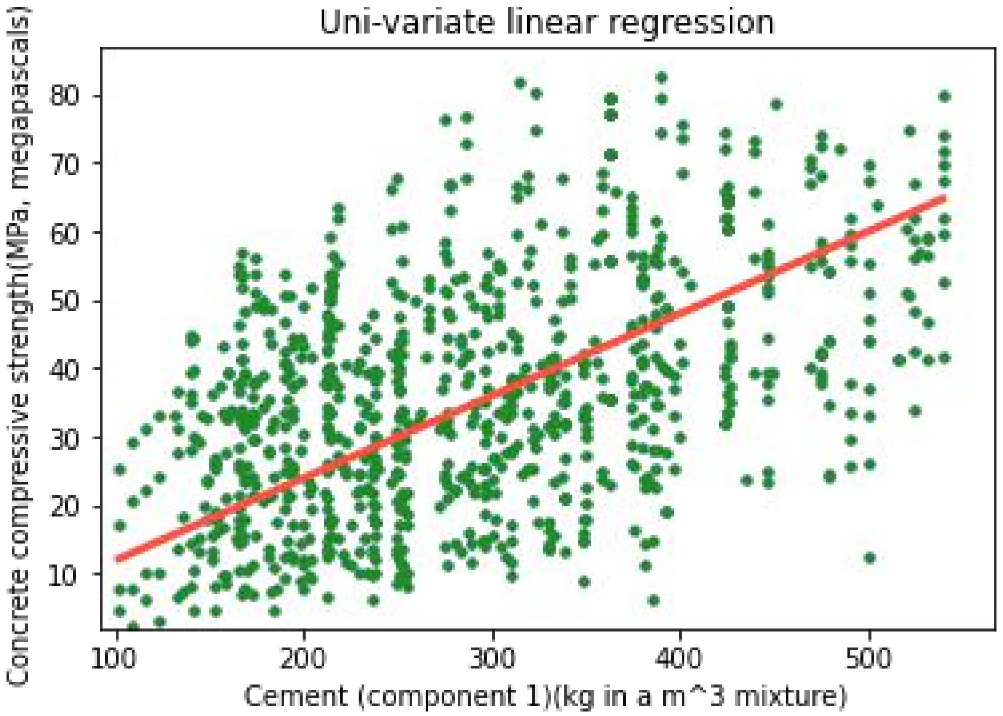
2.1 MSE of training set and test set of each character for later use:

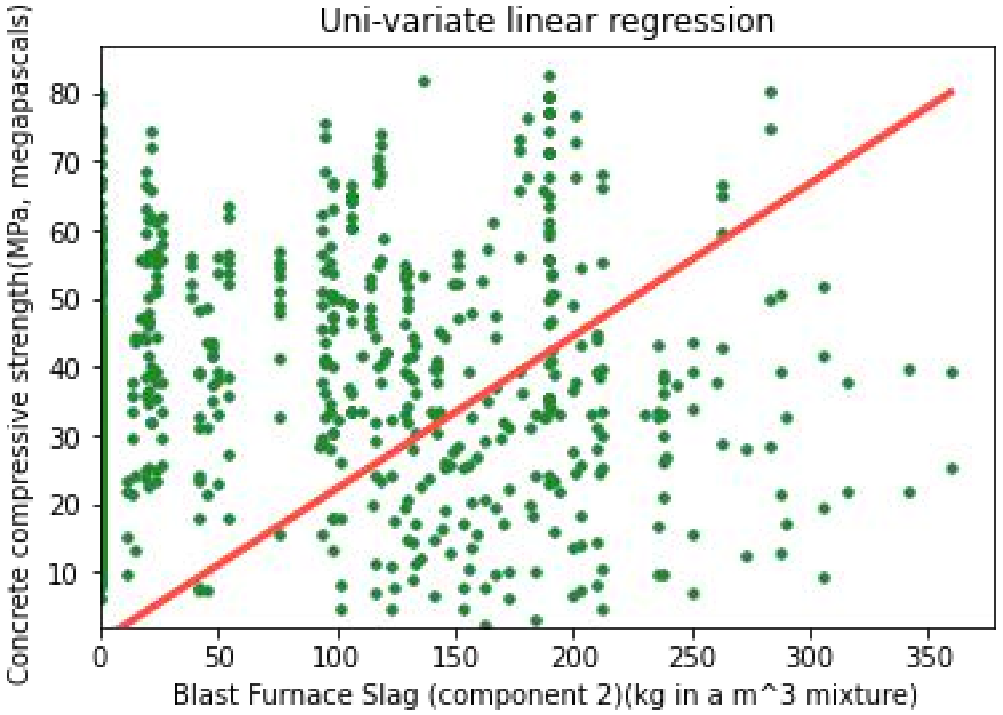
Character	MSE of training set	MSE of test set
Cement (component 1)(kg in a m^3 mixture)	249.423	111.026
Blast Furnace Slag (component 2)(kg in a m^3 mixture)	296.809	173.734
Fly Ash (component 3)(kg in a m^3 mixture)	298.191	144.638
Water (component 4)(kg in a m^3 mixture)	358.233	186.91
Superplasticizer (component 5)(kg in a m^3 mixture)	313.751	146.026
Coarse Aggregate (component 6)(kg in a m^3 mixture)	322.363	165.965
Fine Aggregate (component 7)(kg in a m^3 mixture)	333.462	171.538
Age (day)	270.035	143.722
All characters in Question B	136.3	56.8
45 characters in Question C	185.3	119.9
45 characters after normalized in Question D	7.228348558311763e-05	9.476957712276736e-08
45 characters after standardized in Question D	1.1345330579318404	0.06861343078398412

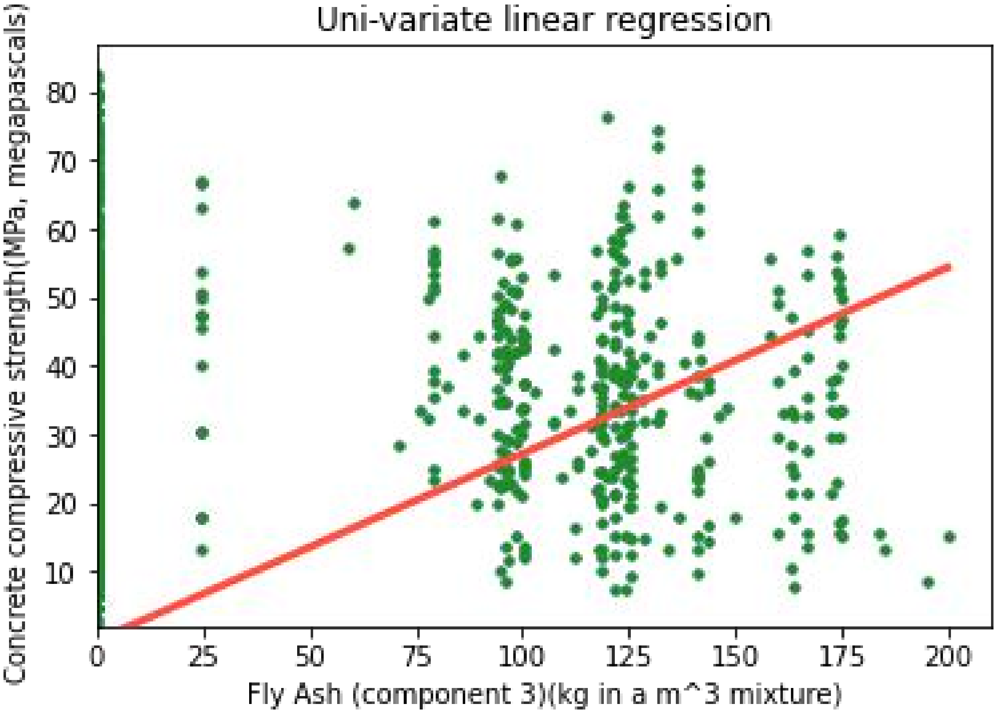
2.2 Variance explained for the response variable of training set and testing set for each feature:

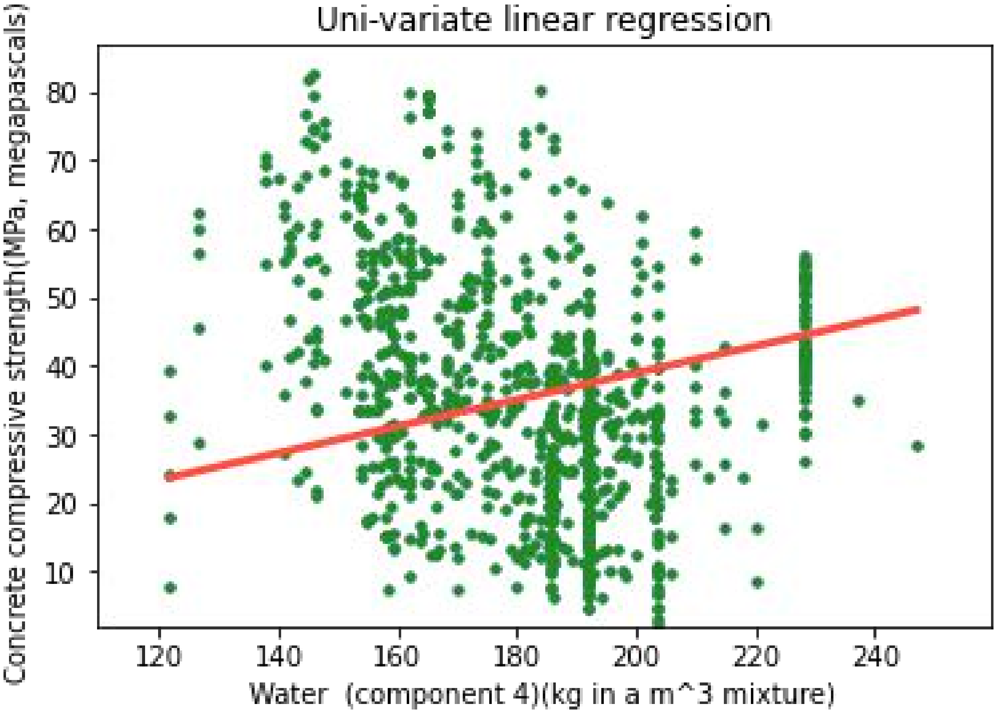
Character	Variance explained of training set	Variance explained of testing set
Cement (component 1)(kg in a m^3 mixture)	0.157	0.625
Blast Furnace Slag (component 2)(kg in a m^3 mixture)	0.012	0.491
Fly Ash (component 3)(kg in a m^3 mixture)	-0.008	0.511
Water (component 4)(kg in a m^3 mixture)	0.157	0.366
Superplasticizer (component 5)(kg in a m^3 mixture)	-0.06	0.506
Coarse Aggregate (component 6)(kg in a m^3 mixture)	-0.09	0.439
Fine Aggregate (component 7)(kg in a m^3 mixture)	-0.127	0.420
Age (day)	0.087	0.514
All characters in Question B	0.637	0.847
45 characters in Question C	0.374	0.595
45 characters after normalized in Question D	-0.095	0.999
45 characters after standardized in Question D	-0.001	0.939

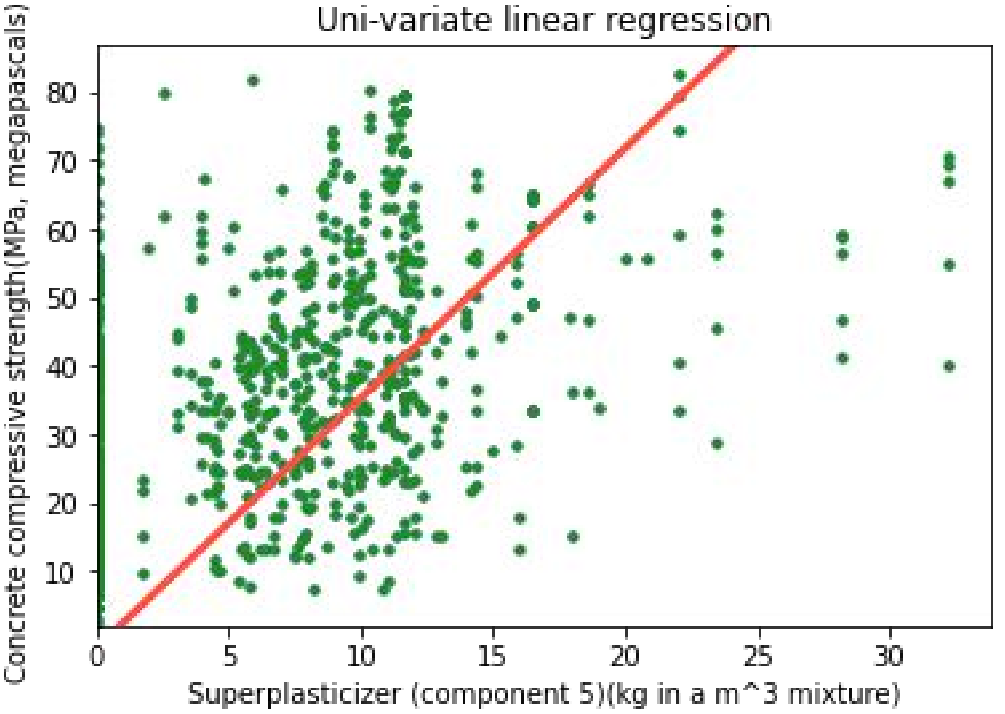
2.3 Plots of my trained uni-variate model on top of scatterplots of the training data used:

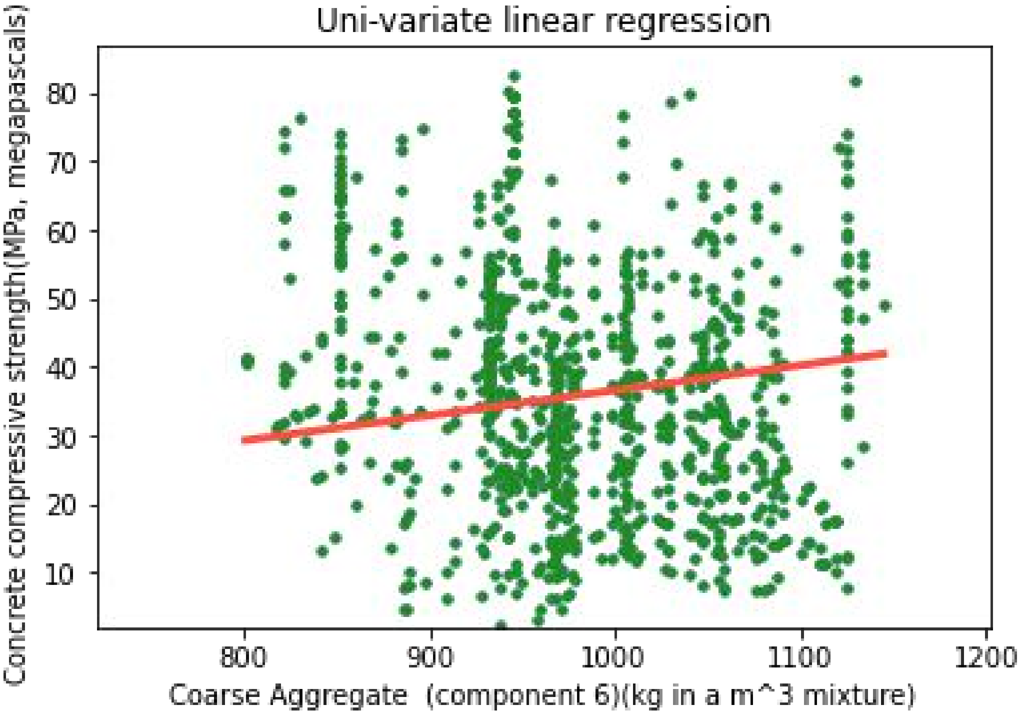

Uni-variate linear regression
Concrete compressive strength(MPa, megapascals)
80
70
60
50
40
30
20
10
100
200
300
400
500
Cement (component 1)(kg in a m^3 mixture)

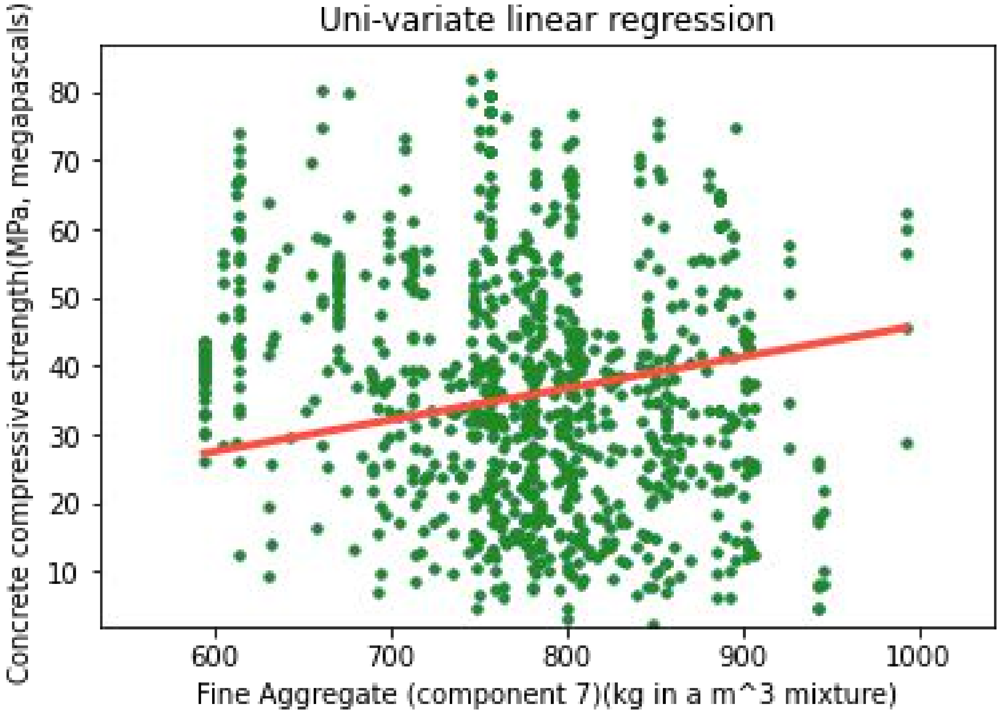

Uni-variate linear regression
Concrete compressive strength(MPa, megapascals)
80
70
60
50
40
30
20
10
0
50
100
150
200
250
300
350
Blast Furnace Slag (component 2)(kg in a m^3 mixture)

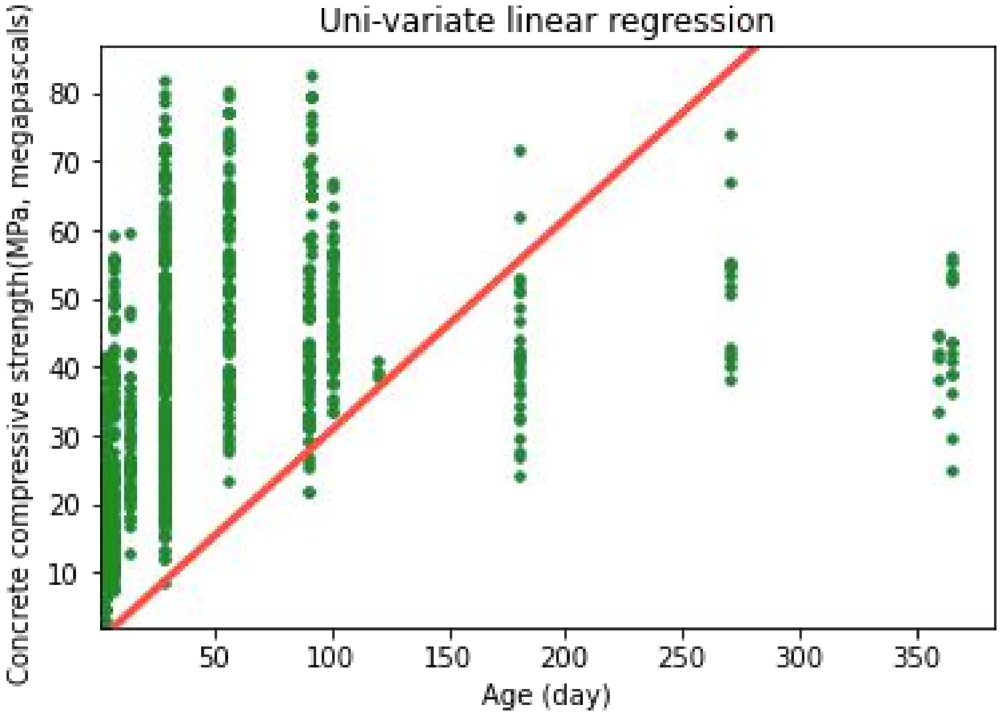

Uni-variate linear regression
Concrete compressive strength(MPa, megapascals)
Fly Ash (component 3)(kg in a m^3 mixture)
10
20
30
40
50
60
70
80
0
25
50
75
100
125
150
175
200


Uni-variate linear regression
Concrete compressive strength(MPa, megapascals)
Water (component 4)(kg in a m^3 mixture)
10
20
30
40
50
60
70
80
120
140
160
180
200
220
240


Uni-variate linear regression
Concrete compressive strength(MPa, megapascals)
10
20
30
40
50
60
70
80
0
5
10
15
20
25
30
Superplasticizer (component 5)(kg in a m^3 mixture)


Uni-variate linear regression
Concrete compressive strength(MPa, megapascals)
10
20
30
40
50
60
70
80
800
900
1000
1100
1200
Coarse Aggregate (component 6)(kg in a m^3 mixture)





3.Discussion

3.1Describe how the different models compared in performance on the training data. Did the same models that performed well on the training data do well on the testing data?

We will have a form which is sorted by MSE of training data as followed:

Character	MSE of training set	MSE of test set
45 characters after normalized in Question D	0.0000723	9.48E-08
45 characters after standardized in Question D	1.134533058	0.068613431
All characters in Question B	136.3	56.8
45 characters in Question C	185.3	119.9
Cement (component 1)(kg in a m^3 mixture)	249.423	111.026
Coarse Aggregate (component 6)(kg in a m^3 mixture)	270.035	165.965
Fine Aggregate (component 7)(kg in a m^3 mixture)	296.809	171.538
Water (component 4)(kg in a m^3 mixture)	298.191	186.91
Superplasticizer (component 5)(kg in a m^3 mixture)	313.751	146.026
Age (day)	322.363	143.722
Blast Furnace Slag (component 2)(kg in a m^3 mixture)	333.462	173.734
Fly Ash (component 3)(kg in a m^3 mixture)	358.233	144.638

Then it's not hard to conclude that normalized model with 45 characters has the outstanding performance on the training data. Besides, the 2nd and 3rd are better than those who has only one character. Therefore, the more we pre-process data on the right track, the more accuate it will be; the more characters to fit, the less loss it will has.

Most of models performed well on both the training data and testing data. However, for Blast Furnace Slag, it is different. Generally speaking, the performance of the model training set and the performance of the test set are not positively correlated, which means we cannot predict MSE of test set by checking MSE of training set.

3.2 Describe how the coefficients of the uni-variate models predicted or failed to predict the coefficients in the multi-variate model(s).

For coefficients of the uni-variate models and multi-variate models is as followed:

Character	Uni-variate m	Multi-variate m	MSE of training set
Cement (component 1)(kg in a m^3 mixture)	0.119940925	2.91178E-05	249.423
Blast Furnace Slag (component 2)(kg in a m^3 mixture)	0.035438781	0.102119833	292.351
Fly Ash (component 3)(kg in a m^3 mixture)	-0.029389575	0.07341922	298.191

Water (component 4)(kg in a m^3 mixture)	0.198964897	0.070304463	358.233
Superplasticizer (component 5)(kg in a m^3 mixture)	0.151670688	-0.051954772	313.751
Coarse Aggregate (component 6)(kg in a m^3 mixture)	0.151670688	0.018543999	322.363
Fine Aggregate (component 7)(kg in a m^3 mixture)	0.046040219	-0.004378694	333.462
Age (day)	0.10863231	0.009997803	270.035

After sorted by Uni-variate m, we can get:

Character	Uni-variate m	Multi-variate m	MSE of training set
Cement (component 1)(kg in a m^3 mixture)	-0.029389575	2.91178E-05	249.423
Blast Furnace Slag (component 2)(kg in a m^3 mixture)	0.035438781	0.102119833	292.351
Fly Ash (component 3)(kg in a m^3 mixture)	0.046040219	0.07341922	298.191
Water (component 4)(kg in a m^3 mixture)	0.10863231	0.070304463	358.233
Superplasticizer (component 5)(kg in a m^3 mixture)	0.119940925	-0.051954772	313.751
Fine Aggregate (component 7)(kg in a m^3 mixture)	0.151670688	-0.004378694	333.462
Coarse Aggregate (component 6)(kg in a m^3 mixture)	0.151670688	2.91178E-05	322.363
Age (day)	0.198964897	0.009997803	270.035

If We can utilize uni-variate m to predict multi-variate m, the order of multi-variate m will be sorted ascending from top to bottom. However, the fact is multi-variate m do not have that order. Therefore, it’s failed for uni-variate to predict the latter. Maybe because of difference of the dimension between uni-variate model and multi-variate model. The conclusion still works after we added quadratic terms, standardlized or normalized.

3.3 Draw some conclusions about what factors predict concrete compressive strength. What would you recommend to make the hardest possible concrete?

1)In a **multi-variate model**, the value of coefficience m might reflect how much it can contribute to concrete compressive strength. After checking the coefficience m in multi-variate model, the rank of factors for predicing concrete compressive strength should be:

Character	Uni-variate m	Multi-variate m	MSE of training set
Blast Furnace Slag (component 2)(kg in a m^3 mixture)	0.035438781	0.07341922	292.351
Fly Ash (component 3)(kg in a m^3 mixture)	0.046040219	0.070304463	298.191
Water (component 4)(kg in a m^3 mixture)	0.10863231	0.018543999	358.233
Superplasticizer (component 5)(kg in a m^3 mixture)	0.119940925	0.009997803	313.751
Coarse Aggregate (component 6)(kg in a m^3 mixture)	0.151670688	2.91178E-05	322.363
Fine Aggregate (component 7)(kg in a m^3 mixture)	0.151670688	-0.004378694	333.462
Age (day)	0.198964897	-0.051954772	270.035
Cement (component 1)(kg in a m^3 mixture)	-0.029389575	0.102119833	249.423

2) In a **uni-variate model,** the MSE for predicting concrete compressive strength should be taken into consideration as well. After **standardlized(For this question I choose standardlize data)** all character’s value. Now we can get:

Character	Coefficience m’s value	MSE of training	MSE of testing
Cement (component 1)(kg in a m^3 mixture)	0.11984403124750186	1.136	0.06
Blast Furnace Slag (component 2)(kg in a m^3 mixture)	0.1197978505086127	1.133	0.037
Fly Ash (component 3)(kg in a m^3 mixture)	0.11965624418599627	1.156	0.101
Water (component 4)(kg in a m^3 mixture)	0.11936413643961247	1.192	0.113
Superplasticizer (component 5)(kg in a m^3 mixture)	0.11958043761638787	1.069	0.087
Coarse Aggregate (component 6)(kg in a m^3 mixture)	0.11922305127728752	1.206	0.094
Fine Aggregate (component 7)(kg in a m^3 mixture)	0.11907346721499563	1.158	0.037
Age (day)	0.11875831948894204	1.196	0.058

After sorted by coefficience m in a descending order from top to bottom, now we can have:

Character	**Coefficience m’s value**	MSE of training	MSE of testing
Cement (component 1)(kg in a m^3 mixture)	0.119844031	1.136	0.06
Blast Furnace Slag (component 2)(kg in a m^3 mixture)	0.119797851	1.133	0.037
Fly Ash (component 3)(kg in a m^3 mixture)	0.119656244	1.156	0.101

Superplasticizer (component 5)(kg in a m^3 mixture)	0.119580438	1.069	0.087
Water (component 4)(kg in a m^3 mixture)	0.119364136	1.192	0.113
Coarse Aggregate (component 6)(kg in a m^3 mixture)	0.119223051	1.206	0.094
Fine Aggregate (component 7)(kg in a m^3 mixture)	0.119073467	1.158	0.037
Age (day)	0.118758319	1.196	0.058

After sorted by MSE of training in a ascending order from top to bottom, now we have:

Character	Coefficience m's value	**MSE of training**	MSE of testing
Superplasticizer (component 5)(kg in a m^3 mixture)	0.119580438	1.069	0.087
Blast Furnace Slag (component 2)(kg in a m^3 mixture)	0.119797851	1.133	0.037
Cement (component 1)(kg in a m^3 mixture)	0.119844031	1.136	0.06
Fly Ash (component 3)(kg in a m^3 mixture)	0.119656244	1.156	0.101
Fine Aggregate (component 7)(kg in a m^3 mixture)	0.119073467	1.158	0.037
Water (component 4)(kg in a m^3 mixture)	0.119364136	1.192	0.113
Age (day)	0.118758319	1.196	0.058
Coarse Aggregate (component 6)(kg in a m^3 mixture)	0.119223051	1.206	0.094

To encapsulate, Cement (component 1)(kg in a m^3 mixture), Blast Furnace Slag (component 2)(kg in a m^3 mixture), Fly Ash (component 3)(kg in a m^3 mixture) , Superplasticizer (component 5)(kg in a m^3 mixture) and Water (component 4)(kg in a m^3 mixture) are very essential for people to predict concrete compressive strength.

I will highly recommend consider using better cement to improve concrete compressive strength, it worths!

3.4 if you include comparisons to the results from normalized or standardized data

3.5 if you include comparisons to the results from your quadratic model

Finished

Quotation:

[1]https://www.sciencedirect.com/topics/materials-science/compressive-strength#:~:text=Compressive%20strength%20can%20be%20defined,the%20characteristics%20of%20the%20concrete.