CSE514 Programming Assignment 1 Report

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Introduction

Description

The goal of this program is to predict the Concrete Compressive Strength from the usages of different type of ingredients.

I am going form the prediction functions using 3 different regression methods, i.e., Uni-variate linear regression, Multi-variate linear regression, and Multi-variate polynomial regression. In the meantime, I developed way to pre-processing the data by standardizing each variable, and compare the speed and result of our program.

Details of Algorithms

Whether used stochastic GD?

Stochastic Gradient Descent does help avoid local minimum, but I didn't use that.

Stop criterions

1. When the L2 Norm of the vector of the partial derivatives of parameters (m1, m2... mi, b) is below certain value, the regression stops. Basically, we want to stop the iteration if the gradient descent is too slow.
    - The stop value for the two linear regression models are `0.000001`.
    - For the quadratic model, the stop value is `0.001`.
    - I've tested that if I use smaller value, the number of iterations will exceed the max steps, which is a million.
2. When the number of steps exceeds certain value, the regression stops.
    - The stop value by default is `1000000`, since I want to make sure they will run enough rounds.

Models	Max Steps	Min L2 Norm of Derivatives
Univariate (Standardized)	1000000	0.000001
Univariate (Non-Standardized)	1000000	0.000001
Multivariate (Standardized)	1000000	0.000001
Multivariate (Non-Standardized)	1000000	0.000001
Quadratic (Standardized)	1000000	0.001
Quadratic (Non-Standardized)	1000000	0.001

Learning rate

I make it changing dynamically regarding the change of loss between each iteration using method `update_alpha`. When the loss goes up, I reduce the learning rate by `50%`, otherwise increase it by `1%`.

The initial value differs among each models and depends on whether Data Pre-Processing is applied. With Pre-Processing, I set it to somewhere between `0.000001` and `0.0000001`. The value also works for data without Pre-Processing, except for the last model, Multi-Variate Polynomial Regress, whose loss value explodes when the learning rate is too big (it goes too far in GD), so I have to set it to `0.0000000001`.

Models	Learning rate
Univariate (Standardized)	0.000001
Univariate (Non-Standardized)	0.000001
Multivariate (Standardized)	0.000001
Multivariate (Non-Standardized)	0.000001
Quadratic (Standardized)	0.000001
Quadratic (Non-Standardized)	0.0000000001

Pseudo Code

Regression

1. The number of feature is **8**; the number of training sample is **900**.
2. `X` = Certain column (vector) or the entire matrix of training feature from the data sheet. Then, we transform it to **900 * 1** or **900 * 8** matrix depending on which model we are using.
3. `Y` = The last column of the data sheet, turn it into **900 * 1** matrix.
4. If this is the Multi-Variate Polynomial Regression, then, append to the right side of X the result of the element-wise multiplication of each feature vectors, which are the **36** quadratic terms.

5. Append a vector of ones to the right end of `X`, for the multiplication with the constant term. (Finally the `X` matrix is either **900 * 2** for model 1, or **900 * 9** for model 2, or **900 * 45** for the quadratic model).
6. `MB` = A **2 * 1**, or **9 * 1**, or **45 * 1** matrix depends on which model we are using, whose last value is the constant term, and the rest are for the linear and quadratic terms.
7. Initialize `LOSS`, `L2 Norm of Derivatives` to **infinity**, `STEPS` to **0**.
8. **WHILE** `L2 Norm of Derivatives` > `StopValue` **and** `STEPS` < `STOP_STEPS`:
    1. `DERIVATIVES` = Calculate the partial derivatives of each parameters in the matrix way. It is a **1** row horizontal matrix.

       (Credit: https://vxy10.github.io/2016/06/25/lin-reg-matrix/)
    2. Apply the learning rate to elements in `DERIVATIVES`. Do element-wise subtraction between `MB` and `DERIVATIVES.T`

       That is, `MB` = `MB` - `DERIVATIVES.T` * `LEARNING_RATE`
    3. `STEPS` += 1
    4. `L2 Norm of Derivatives` = Calculate L2 Norm of `DERIVATIVES`
    5. `NEW LOSS` = Calculate the loss using updated parameters.
    6. Increase `LEARNING RATE` by **0.01** if `NEW LOSS` < `LOSS`, otherwise reduce it by half.
    7. `LOSS` = `NEW LOSS`
9. **RETURN** `MB`.

Additional steps if we do data pre-processing

I am using the **scaling (min-max normalization)** method.

After Step.5 in Regression:

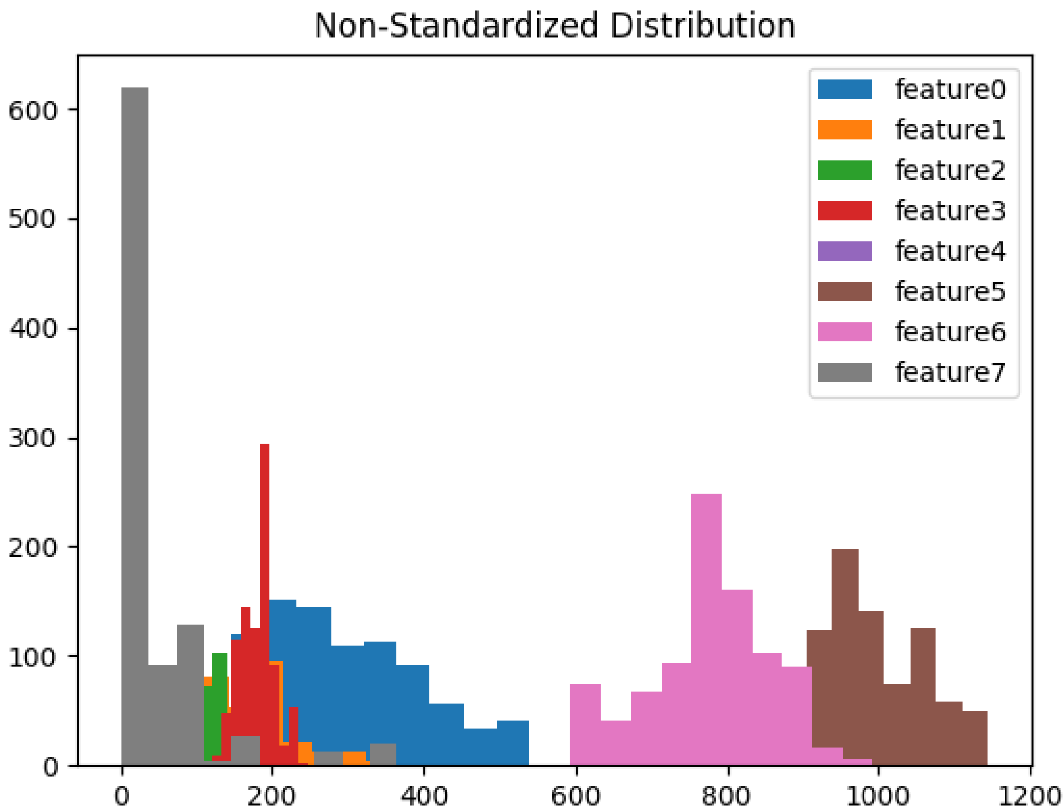
1. `Scales` = [ ]
2. For each columns in `X`, except the last one:
    1. Find the `min` and `max` value in it.
    2. Update each value `v` by `v` = (`v` - `min`) / (`max` - `min`)
    3. Now the data distributed within **0** and **1**.
    4. Append `min` and `max` to `Scales` so that we can properly scale value in the test data set.
3. **Return** the new `X` and `Scales`

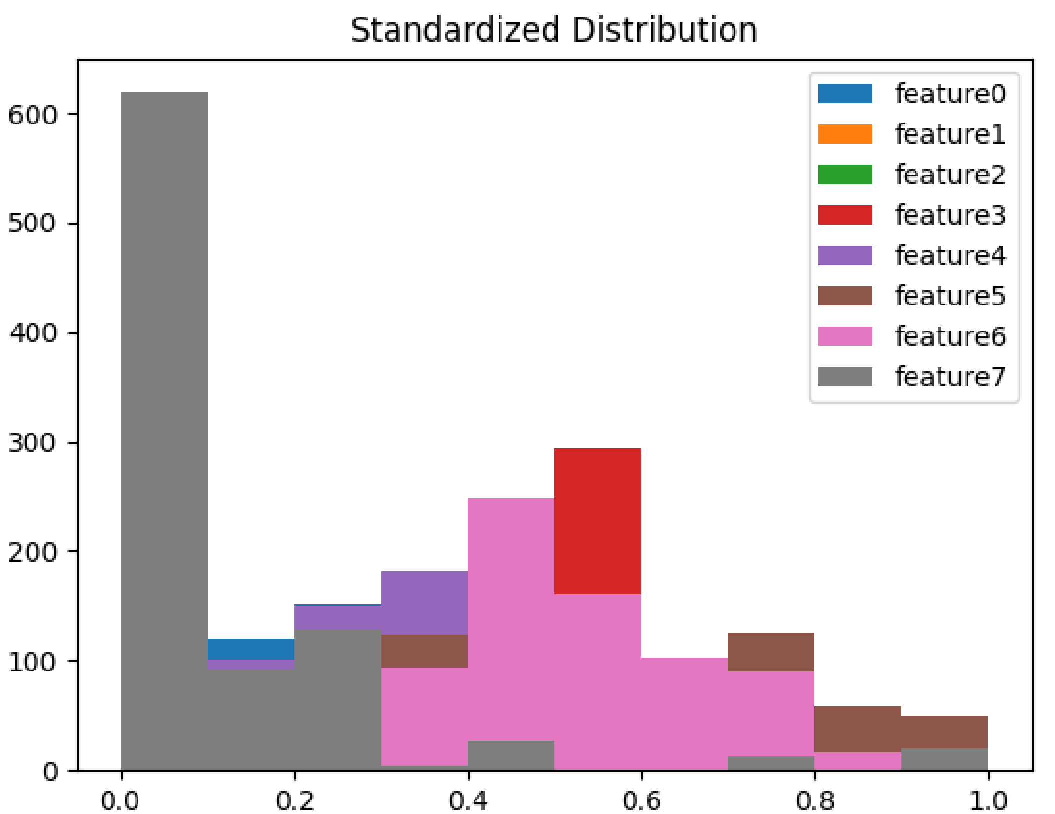
(+2 bonus pts) Description of the Quadratic Model

See above.

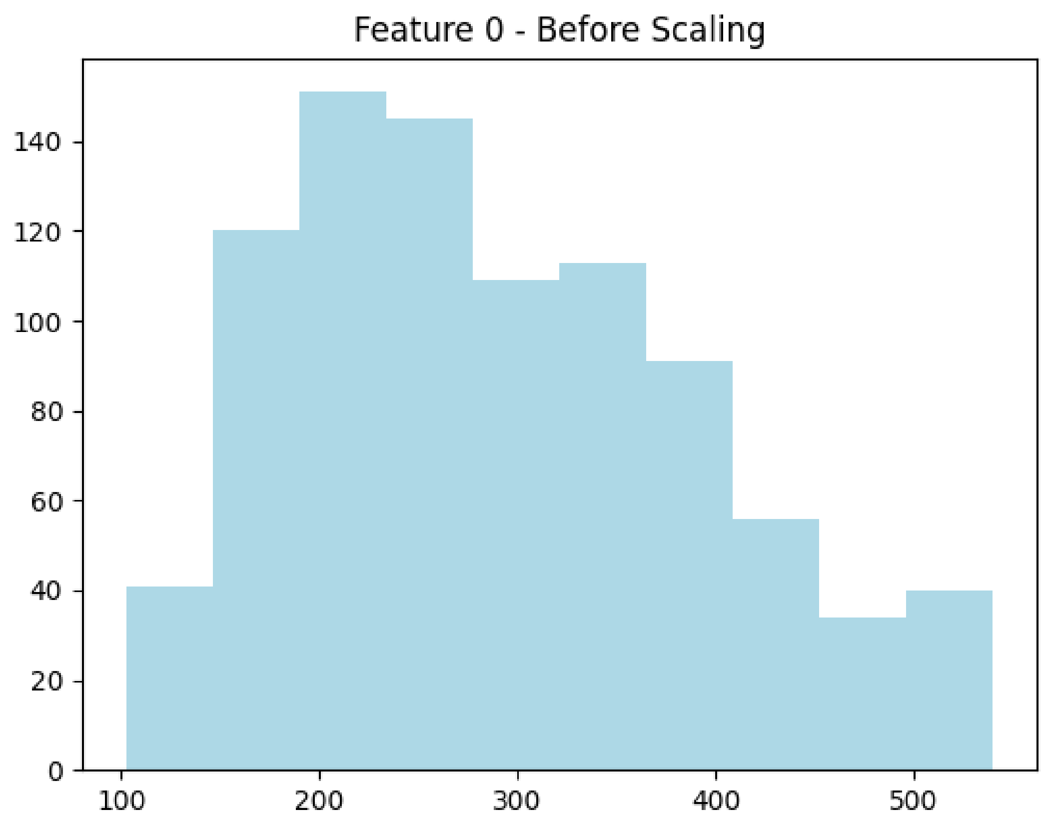
(+4 bonus pts) Description of Data Standardization

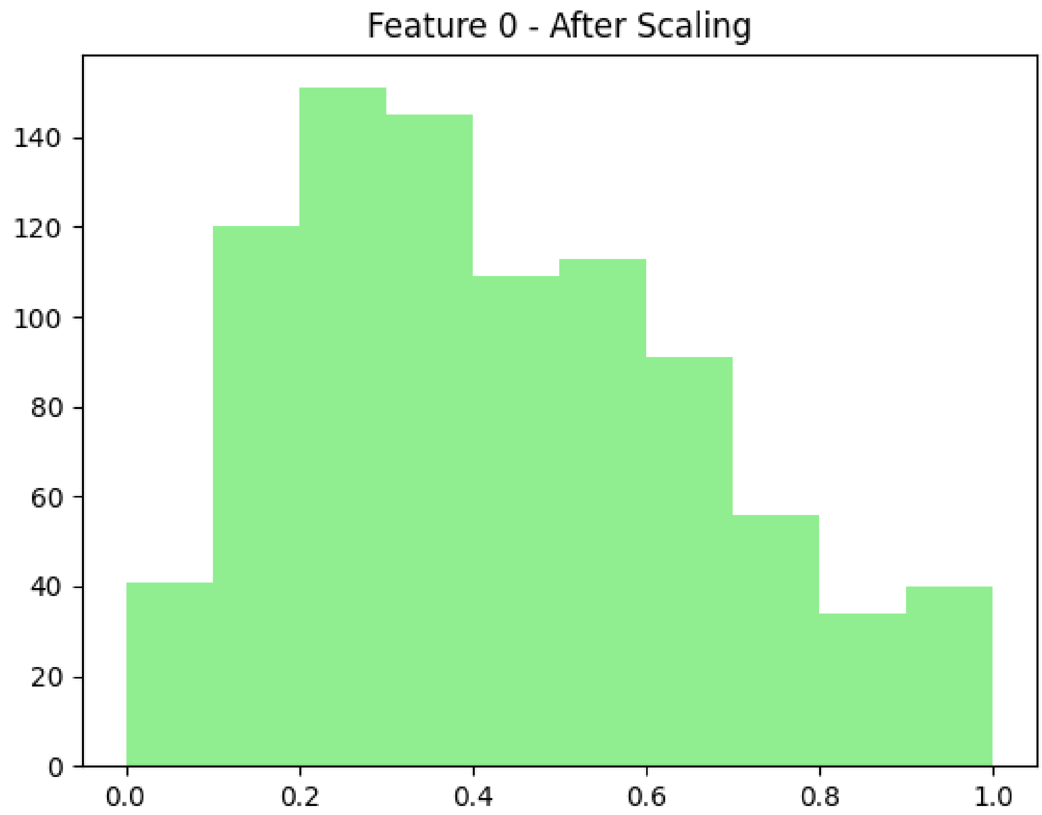
I applied scaling (min-max normalization) to each row of features, to make them fit in between 0 and 1. Since all the data are ranged in [0,1], the gradient decent using single learning rate in multi-variate models is much faster and works better. The following 2 histograms of the distribution of all features combined, shows that all features are on the same scale after standardization.


Non-Standardized Distribution
feature0
feature1
feature2
feature3
feature4
feature5
feature6
feature7
0
100
200
300
400
500
600
0
200
400
600
800
1000
1200


Standardized Distribution
feature0
feature1
feature2
feature3
feature4
feature5
feature6
feature7
0
100
200
300
400
500
600
0.0
0.2
0.4
0.6
0.8
1.0

In the mean time, the pattern of features won't change before and after the scaling so we won't lost information in the process. Take the diagram of feature 0 as example, shown below:





Results

Variance explained of models on the training dataset

The training automatically stops when the L2 Norm of derivatives reaches the stop value. Although the result seems similar on both training on pre-processed and non-preprocess data, the iterations elapsed are significantly different. The iterations of training on pre-processed data are no more than 5000; for uni-variate models; no more than 100000 for the multi-variate linear model; and no more than 600000 for the quadratic model. However, almost all training on non-preprocessed data exceeded the maximum iterations while the result was still inferior to those from pre-processed. So data pre-processing can at least fasten the training speed.

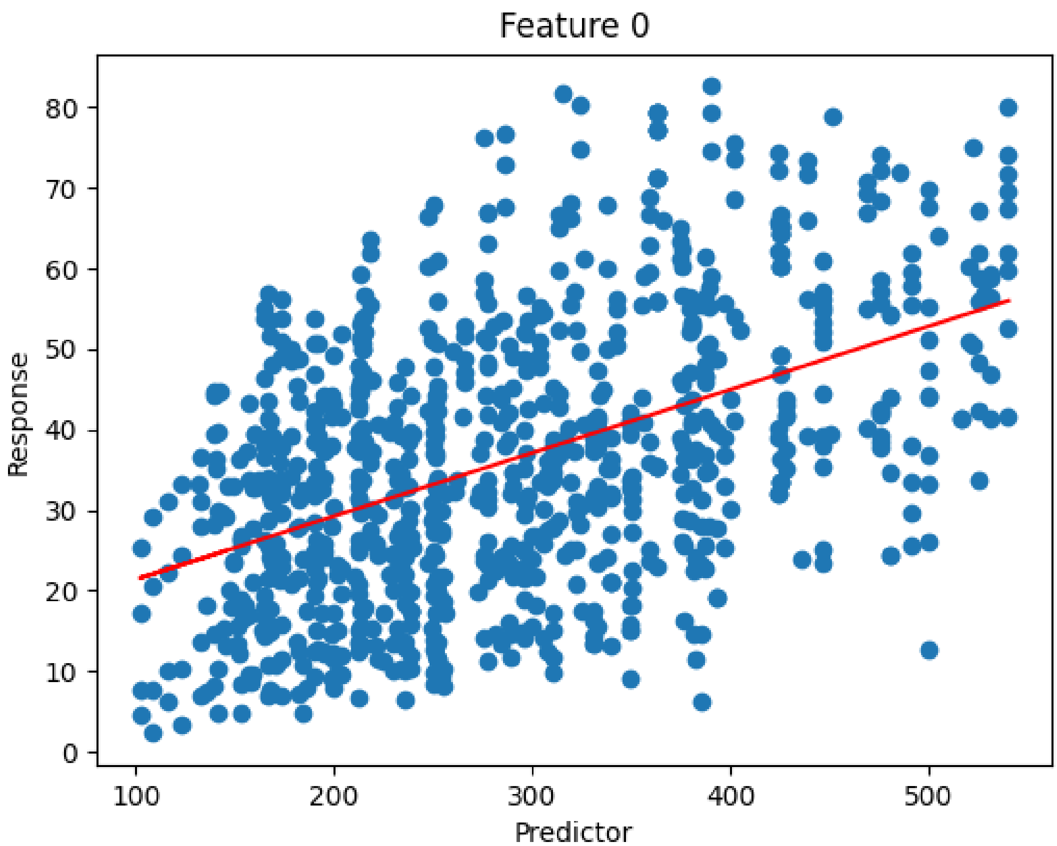
Models	Pre-Processed	Non-Pre-Processed
Uni-Variate Linear Regression - Feature.0	0.22825858392552245	0.2277804149950582
Uni-Variate Linear Regression - Feature.1	0.017208971265118556	0.0172089712629645
Uni-Variate Linear Regression - Feature.2	0.002035355116008719	0.0020353551148349913
Uni-Variate Linear Regression - Feature.3	0.0870741625546625	0.03748129894822072
Uni-Variate Linear Regression - Feature.4	0.17428080158691384	0.17428080158695125
Uni-Variate Linear Regression - Feature.5	0.038466583708890334	-0.0863160383151611
Uni-Variate Linear Regression - Feature.6	0.03228636782791372	-0.11561388393254313
Uni-Variate Linear Regression - Feature.7	0.1113823961381637	0.11138239613721601
Multi-Variate Linear Regression	0.6127199839036626	0.6127141689062416
Multi-Variate Polynomial Regression	0.8079087791510478	0.7867129699118943

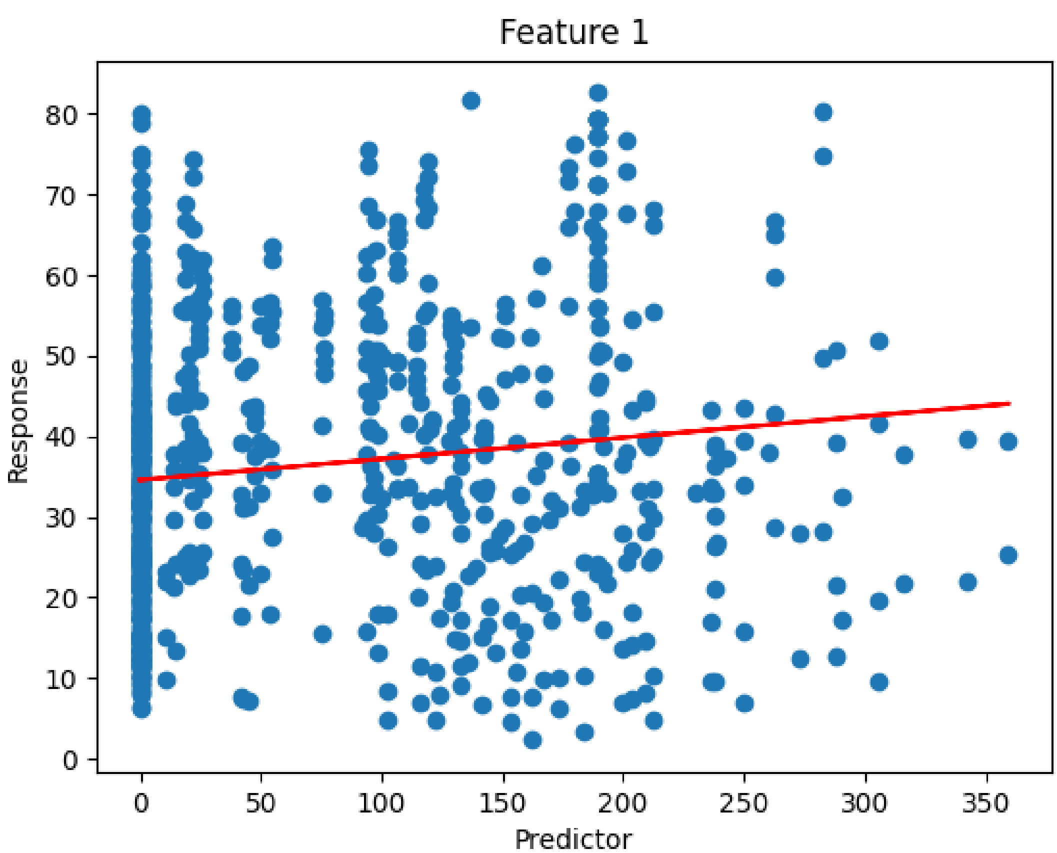
Variance explained of models on the testing set

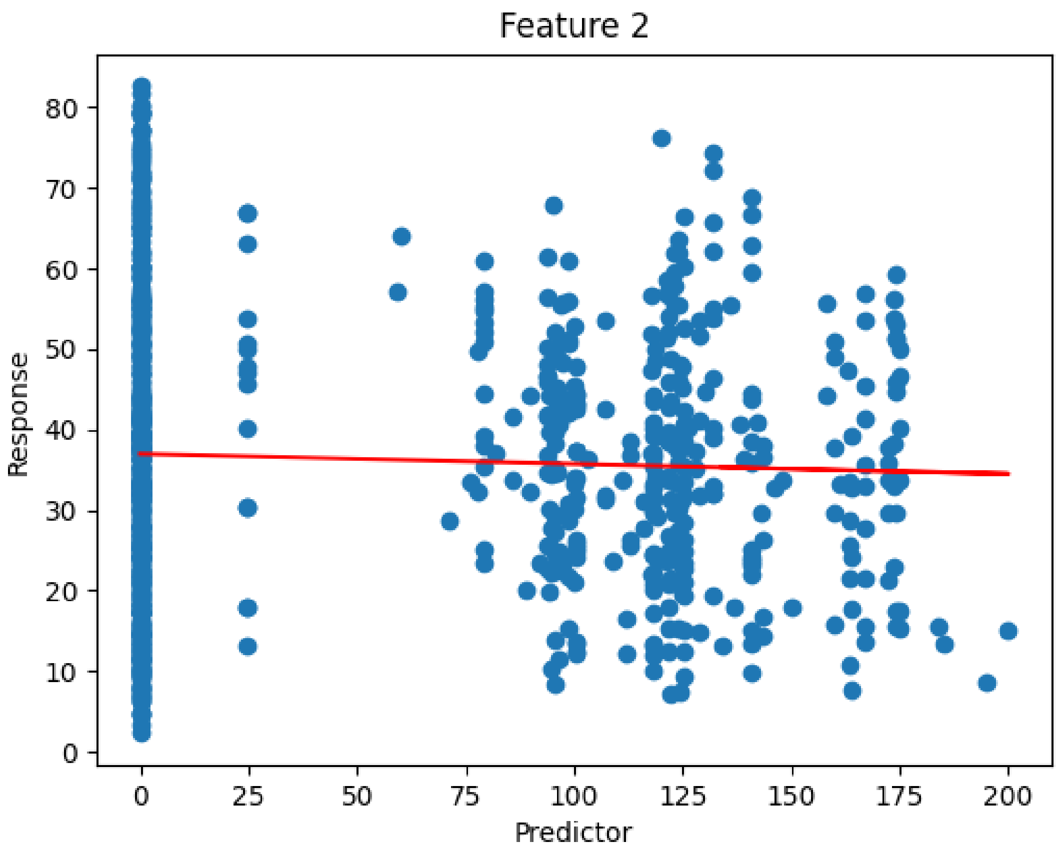
The result for uni-variate models are inconsistent, but for the multi-variate linear and polynomial models, the result is significantly better than uni-variate models.

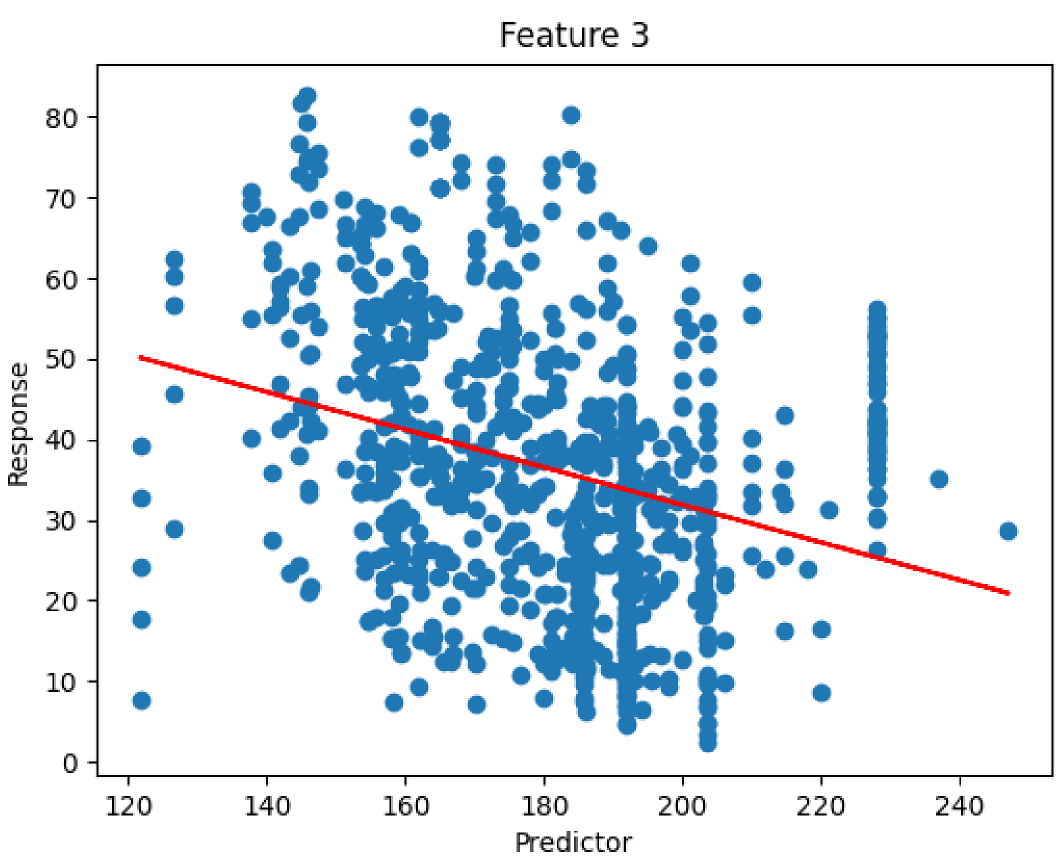
Models	Pre-Processed	Non-Pre-Processed
Uni-Variate Linear Regression - Feature.0	0.4354355804392598	0.434876189970022
Uni-Variate Linear Regression - Feature.1	-0.11115955003290523	-0.11115813448037226
Uni-Variate Linear Regression - Feature.2	-0.039987586834406175	-0.03998781370598703
Uni-Variate Linear Regression - Feature.3	-0.07842408402413148	-0.07278655900919406
Uni-Variate Linear Regression - Feature.4	-0.6374844347303614	-0.637484762882583
Uni-Variate Linear Regression - Feature.5	-0.32388437251178415	-0.15129306498166994
Uni-Variate Linear Regression - Feature.6	-0.1759077749792861	-0.18328761221673173
Uni-Variate Linear Regression - Feature.7	-0.05013853815163971	-0.05013783419568929
Multi-Variate Linear Regression	0.5789460184844312	0.5775885231620859
Multi-Variate Polynomial Regression	0.6749234729927985	0.6870487192510564

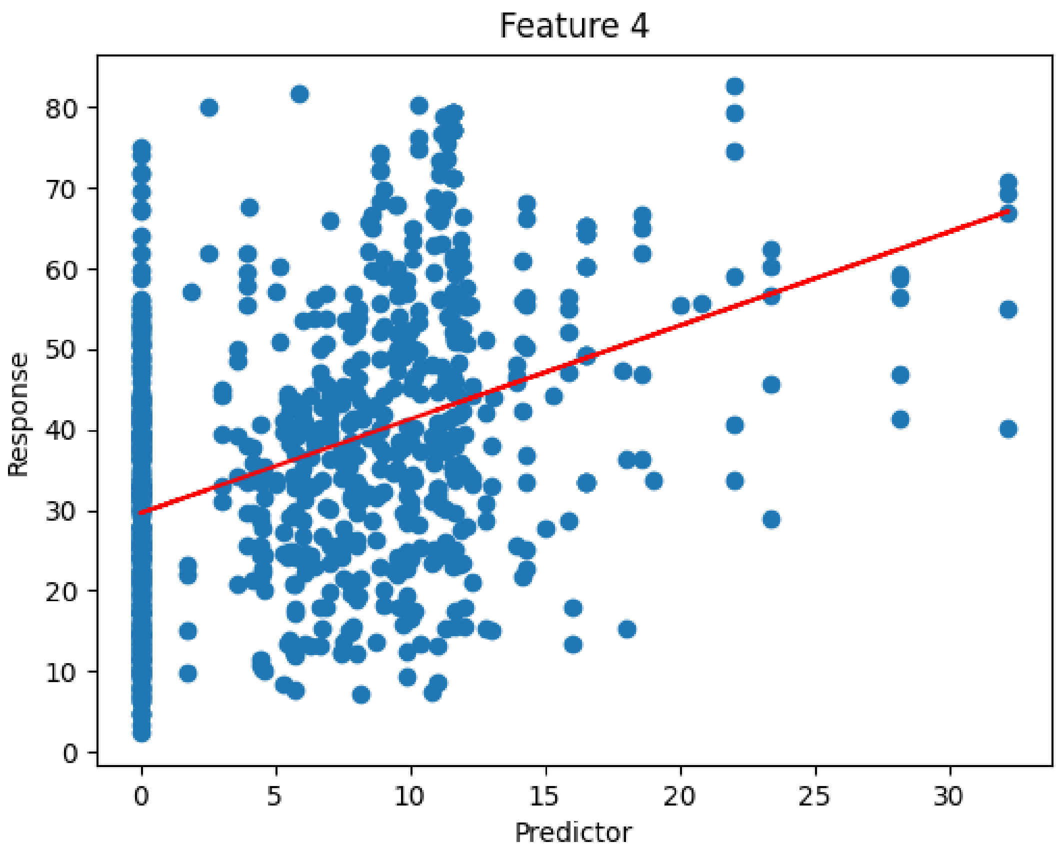
Plots of trained Uni-Variate models (Data is Pre-Processed)

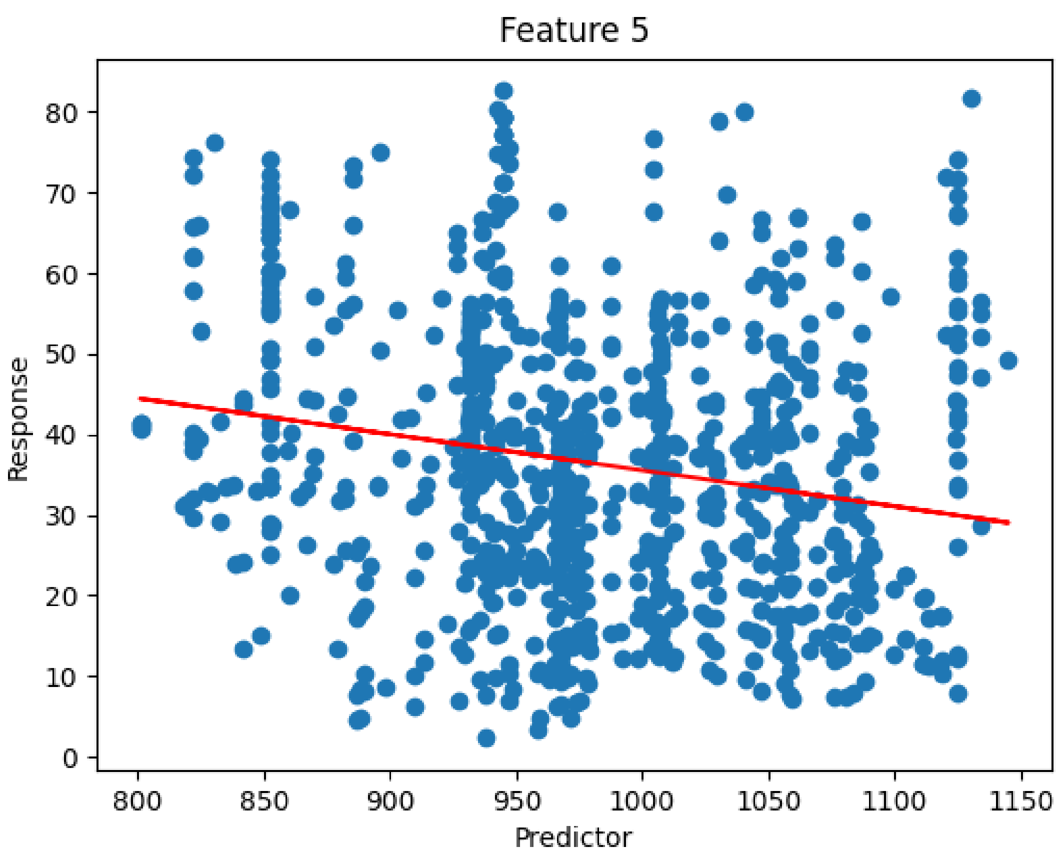


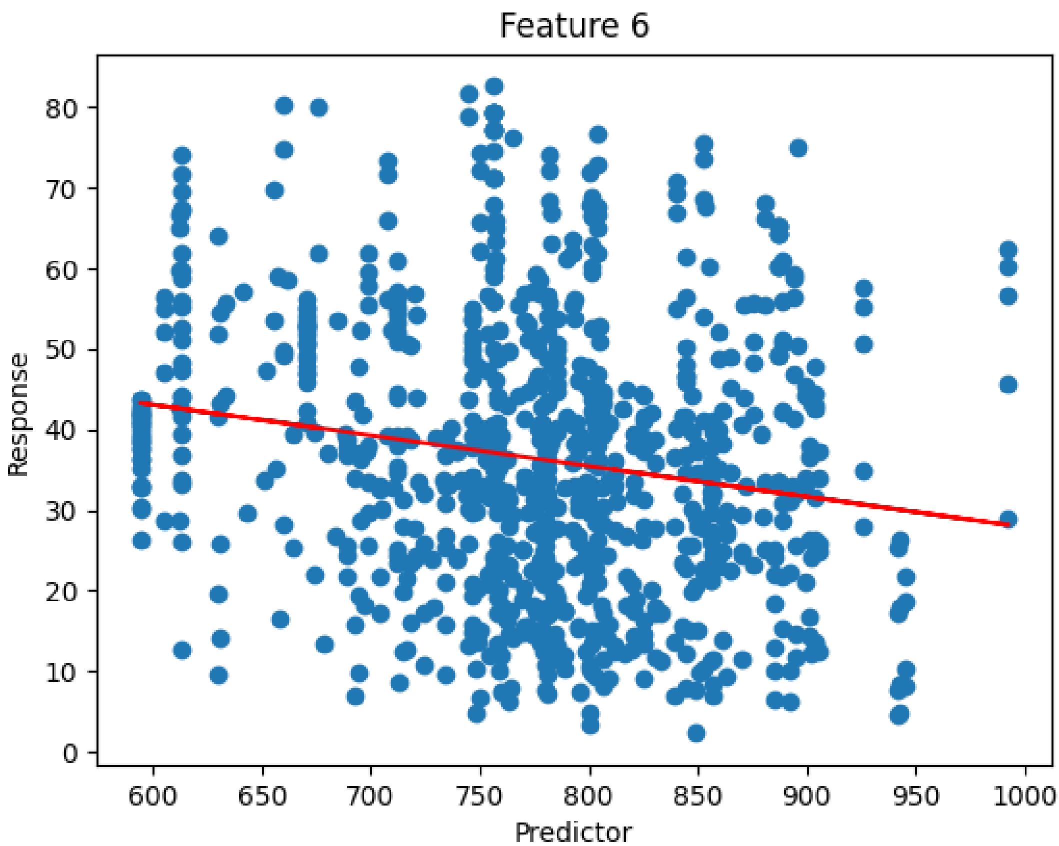


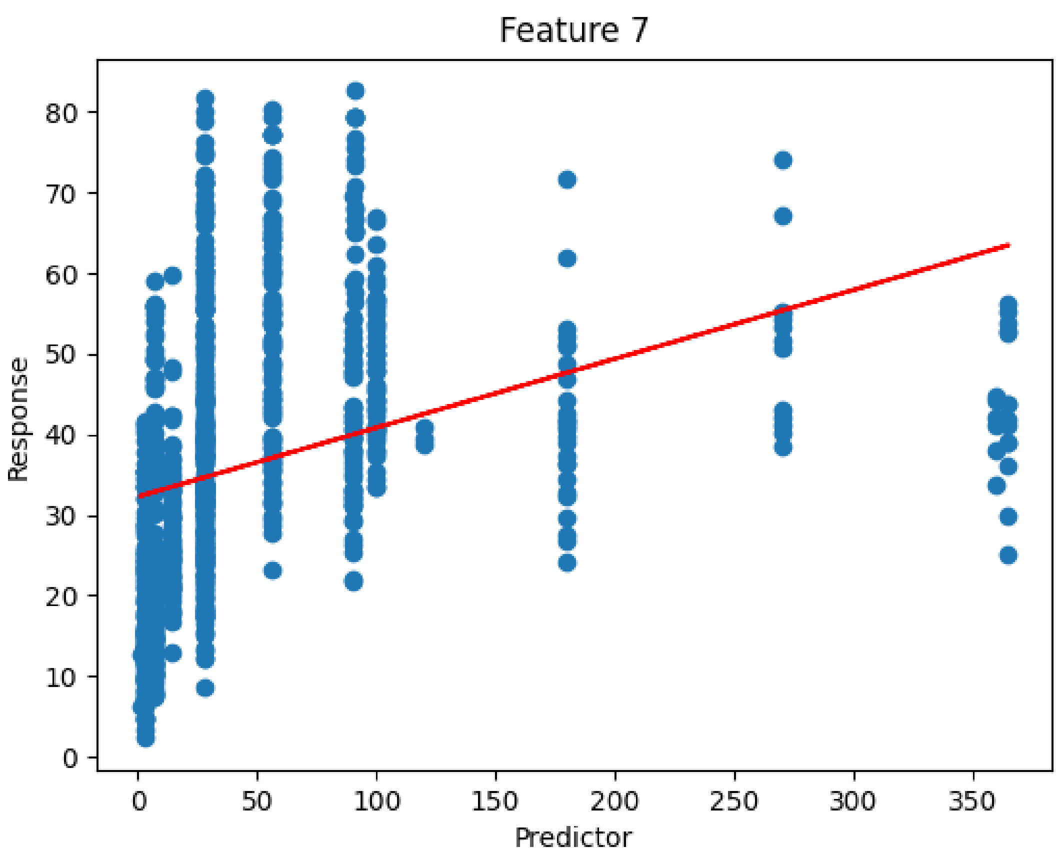

Feature 2
Response
Predictor
0
10
20
30
40
50
60
70
80
0
25
50
75
100
125
150
175
200


Feature 3
Response
Predictor
0
10
20
30
40
50
60
70
80
120
140
160
180
200
220
240


Feature 4
Response
Predictor
0
10
20
30
40
50
60
70
80
0
5
10
15
20
25
30


Feature 5
Response
Predictor
0
10
20
30
40
50
60
70
80
800
850
900
950
1000
1050
1100
1150


Feature 6
Response
Predictor
0
10
20
30
40
50
60
70
80
600
650
700
750
800
850
900
950
1000


Feature 7
Response
Predictor
0
10
20
30
40
50
60
70
80
0
50
100
150
200
250
300
350

(+4 bonus points) if you include results from your quadratic model.

See first two parts of **Results**.

(+4 bonus points) if you include results from using normalized or standardized feature values as input

See first two parts of **Results**.

Discussion

Describe 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

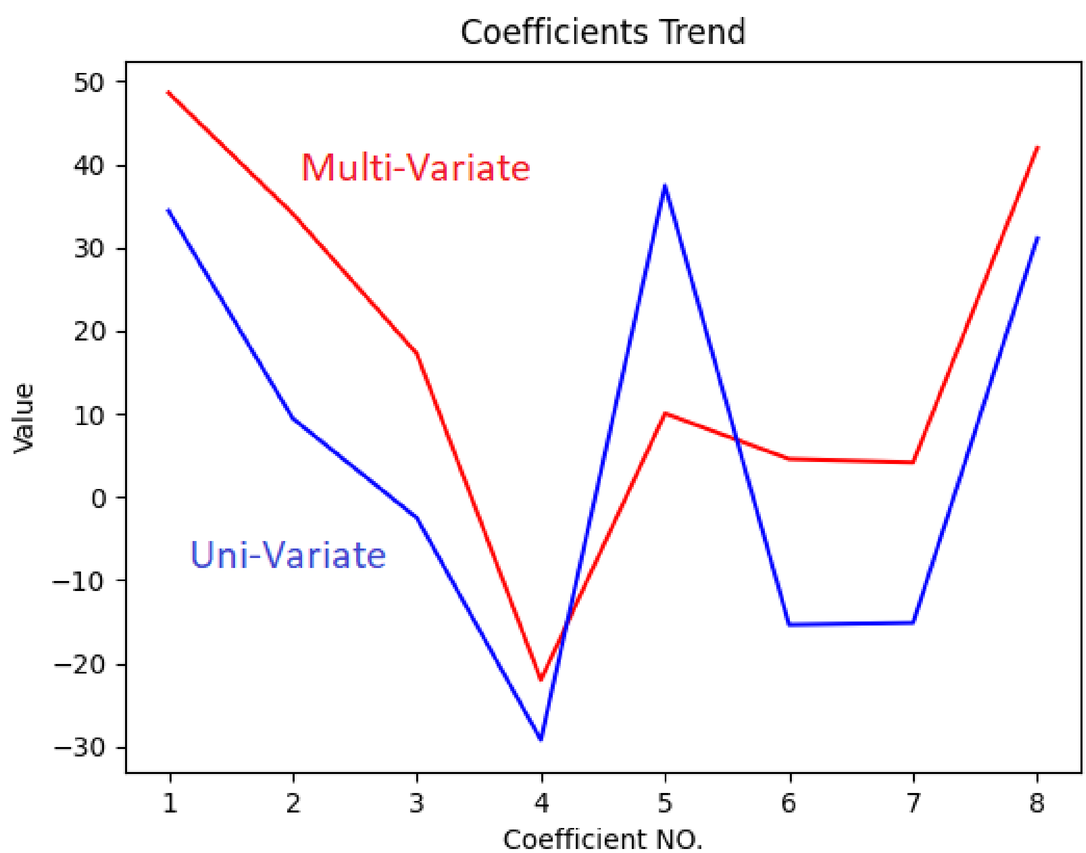
1. The uni-variate models have pretty bad performance on training data, only slightly better than calculating the mean value of the true result.
2. The uni-variate models are unreliable in predicting the testing dataset even if they did well in training data.
3. The multi-variate models (both linear and polynomial) have significantly better performance on both training and testing data, as we can see from the result of calculation of variance explained for different models. These two models have values that are much closer to 1, while the polynomial one is much better (more than 0.8).
4. Both multi-variate models have consistent performance in predicting both training and testing datasets. However, the value explained for testing dataset is slightly worse than the result for training dataset.
5. Without data-preprocessing, however, uni-variate models may be even worse than calculating the average value of the true responses. This may caused by insufficient iterations of model training since they require more iterations based on my observation.

Models	R Square (Pre-Processed)	Iterations	R Square (Non-Pre-Processed)	Iterations
Uni-Variate Linear Regression - Feature.0	0.22825858392552245	1530	0.2277804149950582	1000000
Uni-Variate Linear Regression - Feature.1	0.017208971265118556	1481	0.0172089712629645	1000000
Uni-Variate Linear Regression - Feature.2	0.002035355116008719	1445	0.0020353551148349913	1000000
Uni-Variate Linear Regression - Feature.3	0.0870741625546625	1000000	0.03748129894822072	1000000
Uni-Variate Linear Regression - Feature.4	0.17428080158691384	1000000	0.17428080158695125	1000000
Uni-Variate Linear Regression - Feature.5	0.038466583708890334	1602	-0.0863160383151611	1000000
Uni-Variate Linear Regression - Feature.6	0.03228636782791372	1614	-0.11561388393254313	1000000
Uni-Variate Linear Regression - Feature.7	0.1113823961381637	1000000	0.11138239613721601	1000000
Multi-Variate Linear Regression	0.6127199839036626	13838	0.6127141689062416	1000000
Multi-Variate Polynomial Regression	0.8079087791510478	510753	0.7867129699118943	1000000

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

Note: I am using the coefficients from models trained from pre-processed data.

Feature NO.	Coefficient of each Uni-Variate Linear model	Coefficients of Multi-Variate Linear model
Feature 0	34.41549554	48.61112746
Feature 1	9.45514834	34.08097931
Feature 2	-2.5087669	17.2405404
Feature 3	-29.22722009	-22.00664687
Feature 4	37.47737023	10.03806901
Feature 5	-15.37887138	4.57227349
Feature 6	-15.14577079	4.16281615
Feature 7	31.11197486	41.99221665



Based on the value and the chart, it is clearly that the coefficients from uni-variate models predicts those of multi-variate model. The bigger coefficients in uni-variate models tends to be also bigger in multi-variate model. Each feature is kind of sharing the similar importance in both models.

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

Based on the observation of the coefficients of Multi-Variate Linear Model (the table and figure above), if we want the concrete compressive strength be higher, we would like to put more of those features(factors) with higher and positive coefficients into the concrete.

Based on the observation of the coefficients of Multi-Variate Polynomial Model (the table below, Note: I am using the coefficients from models trained from pre-processed data), which has much better variance explained, we would like to use more features(factors) or combinations that having higher and positive coefficients in the concrete.

Usages of features(factors) or combinations that having coefficients close to 0 are less likely to impact the strength of concrete.

We would want to avoid using too many features(factors) or combinations having significant negative coefficients.

Feature NO. (Or Combination of Features)	Coefficients of Multi-Variate Polynomial Model (Descending)
3	211.851478480
0	197.399327790
26	115.218527760
25	97.153549190
55	85.363021730
56	84.213356410
67	79.972568550
05	62.369067670
16	60.749666560
6	52.753701350
15	50.151554880
34	43.816737730
17	37.888780000
22	37.607817080
02	36.643964390
07	36.258612970
12	35.807631640
7	31.832461640
4	21.470007780
45	21.304594470
01	15.011980260
11	13.198980400
27	12.541397510
47	9.231974300
44	-5.614389830
37	-5.788901930
33	-7.836047510
14	-14.789089770

Feature NO. (Or Combination of Features)	Coefficients of Multi-Variate Polynomial Model (Descending)
46	-15.789359960
00	-16.801119210
57	-26.076445590
23	-26.843424180
24	-27.136023710
06	-39.512876270
13	-57.025922680
36	-67.149415890
1	-68.795554180
35	-69.408419440
04	-72.299290530
77	-82.309432350
66	-88.024438650
5	-126.036367170
03	-175.448358800
2	-230.991769440

(+2 bonus points) if you include comparisons to the results from normalized or standardized data.

See first part of **Discussion**

(+2 bonus points) if you include comparisons to the results from your quadratic model.

See first part of **Discussion**