1

Linear Regression using Machine Learning

Yi Qiang Ji Zhang Biel Galiot Pérez Gerard Villalta Quintana Oriol Miras Robles

Professor: Alex Ferrer Ferre

Aerospace Engineering

Numerical Tools in Machine Learning for Aeronautical Engineering Polytechnic University of Catalonia — BarcelonaTech



Date: 11 May 2021

I. Introduction

Linear regression attempts to model the relationship between two variables by fitting a linear equation to observed data. One variable is considered to be an explanatory variable (data), and the other is considered to be a dependent variable (outcome). It is used to predict values within a continuous range rather than trying to classify them into categories [1] [2].

There are two main types:

• Simple regression: Simple linear regression uses traditional slope-intercept form, where m and n are the variables the algorithm will try to "learn" to produce the most accurate predictions. x represents the input data and y represents the algorithm's prediction.

$$y = mx + n \tag{1}$$

• Multi-variable regression: This is a more complex linear regression. Where w_i represents the coefficients, or weights, that the algorithm model will try to "learn".

$$f(x_i) = \sum_{i=1}^{N} w_i x_j \quad \forall \ i, j \in \mathbb{N}$$
 (2)

and x_j represents the different variables.

II. LINEAR REGRESSION

In order to implement a linear regression predictor, as a first approach, a simple linear regression without an independent parameter n will be implemented and so the model will simply output

$$y = mx (3)$$

Where m is a vector of parameters (weights) and x is the vector of input data. In order to do so, a set of data is randomly generated using the function generateData.

This function is set to generate a quadratic set of data with some error that is artificially added.

Secondly, 25% of the data points are reserved in order to be used to perform the test of our model, while the rest is set to feed the training of the linear regression model. This is done with splitDataTrainAndTest.

Once the data has been separated, the model itself is finally trained, by minimizing the MSE of the data destined to train. Attending to [3], this is done following the following procedure

$$\nabla_{\boldsymbol{w}} MSE_{train} = 0 \tag{4}$$

$$\Rightarrow \nabla_{\boldsymbol{w}} \frac{1}{m} \left\| \hat{\boldsymbol{y}}^{(\text{train})} - \boldsymbol{y}^{(\text{train})} \right\|_{2}^{2} = 0$$
 (5)

$$\Rightarrow \frac{1}{m} \nabla_{\boldsymbol{w}} \left\| \boldsymbol{X}^{(\text{train})} \boldsymbol{w} - \boldsymbol{y}^{(\text{train})} \right\|_{2}^{2} = 0$$
 (6)

$$\Rightarrow \nabla_{\boldsymbol{w}} \left(\boldsymbol{X}^{(\text{train})} \boldsymbol{w} - \boldsymbol{y}^{(\text{train})} \right)^{\top}$$

$$\left(\boldsymbol{X}^{(\text{train})} \boldsymbol{w} - \boldsymbol{y}^{(\text{train})} \right) = 0 \quad (7)$$

$$\Rightarrow \nabla_{\boldsymbol{w}} \left(\boldsymbol{w}^{\top} \boldsymbol{X}^{(\text{train})\top} \boldsymbol{X}^{(\text{train})} \boldsymbol{w} - 2\boldsymbol{w}^{\top} \boldsymbol{X}^{(\text{train})\top} \boldsymbol{y}^{(\text{train})} + \boldsymbol{y}^{(\text{train})\top} \boldsymbol{y}^{(\text{train})} \right) = 0 \quad (8)$$

$$\Rightarrow 2\boldsymbol{X}^{(\text{train})\top}\boldsymbol{X}^{(\text{train})}\boldsymbol{w} - 2\boldsymbol{X}^{(\text{train})\top}\boldsymbol{y}^{(\text{train})} = 0 \quad (9)$$

$$\Rightarrow \boldsymbol{w} = \left(\boldsymbol{X}^{(\text{train})\top}\boldsymbol{X}^{(\text{train})}\right)^{-1}\boldsymbol{X}^{(\text{train})\top}\boldsymbol{y}^{(\text{train})} \quad (10)$$

Which finally leads to the expression used in the ${\tt computeW}$ function

$$\Rightarrow \boldsymbol{w} = \left(\boldsymbol{X}^{(\text{train })\top}\boldsymbol{X}^{(\text{train })}\right)^{-1}\boldsymbol{X}^{(\text{train })\top}\boldsymbol{y}^{(\text{train })}$$
(11)

With the vector of \boldsymbol{w} , the predictor function can be obtained simply by means of equation (3).

Finally the MSE of the predicted vs actual datapoints for the $y^{(\text{train})}$ is computed with the function computeMSE, which in turn uses MATLAB's immse function.

III. K-FOLD CROSS-VALIDATION

Cross-validation techniques are used to train algorithms when the information given by the datasets is not large enough. Thus, splitting this datasets in different permutations of training and test sets allows to reuse the original data and improve the performance of the algorithm.

One of these techniques is K-Fold Cross-Validation. This method splits the dataset in k number of folds, which will create k mutually exclusive subsets, whose union results on the original dataset.

Algorithm 1 KFold Algorithm

- 1: **Define** KFoldXV(\mathbb{D}, A, L, k)
- 2: **Require**: \mathbb{D} , the given dataset, with elements $\boldsymbol{z}^{(i)}$
- 3: **Require**: A, the learning algorithm, seen as a function that takes a dataset as input and outputs a learned function
- 4: **Require**: L, the loss function, seen as a function from a learned function f and an example $z^{(i)} \in \mathbb{D}$ to a scalar $\in \mathbb{R}$
- 5: **Require**: k, the number of folds
- 6: for i from 1 to k do
- 7: $f_i = A(\mathbb{D}\backslash\mathbb{D}_i)$
- 8: for $z^{(j)}$ in \mathbb{D}_i do
- 9: $e_i = L\left(f_i, \boldsymbol{z}^{(j)}\right)$
- 10: end for
- 11: end for

Each of this combinations of test subsets, with their own training subsets (the remaining values for each one) will return an error. The total error of the algorithm is calculated with the mean value of the k number of errors.

$$E = \frac{1}{K} \sum_{i=1}^{K} E_i \tag{12}$$

IV. Results

To begin with, the following report tries random points of a parabolic curve

$$y = x^2 \tag{13}$$

for values of $x \in (-1,1)$

A. Figure 1

MSE plot (mean and standard deviation) based on training set / test set ratio.

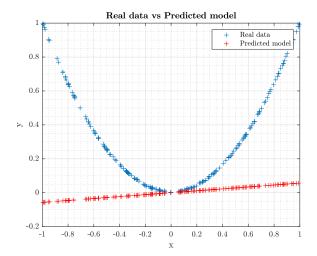


Fig. 1. Real data vs Predicted model

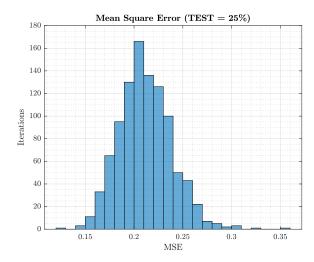


Fig. 2. Histogram for a Test ratio of (25%)

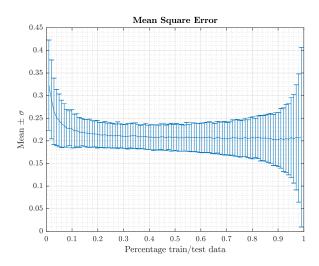


Fig. 3. MSE as a function of the Training/test ratio

B. Figure 2

MSE plot (mean and standard deviation) based on nData for a specific training set / test set ratio value.

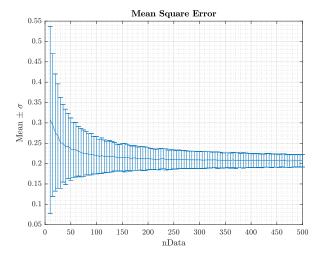


Fig. 4. MSE for a Test ratio of (25%) for different values of nData.

Mean Square Error using k-fold cross validation as a function of nData 35 30 25 10 0 0.02 0.04 0.06 0.08 0.1 0.12 0.14 0.16 MSE

Fig. 7. Histogram as a function of nData for a specific value of folds.

C. Figure 3

MSE plot (mean and standard deviation) based on the number of folds using the k-fold algorithm.

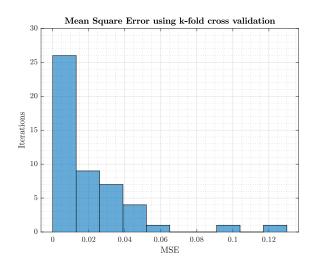


Fig. 5. Histogram as a function of folds using k-fold algorithm.

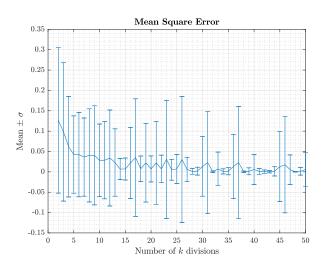


Fig. 6. MSE as a function of folds using k-fold algorithm.

D. Figure 4

MSE plot (mean and standard deviation) based on nData for a specific value of folds.

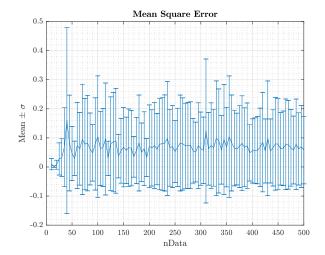


Fig. 8. $\,$ MSE as a function of nData for a specific value of folds.

E. Extra

Same problem with the term constant (i.e. add an unknown bias term b within the parameters to be found). This model is known as affine.

Comparison of the two models (linear and affine)

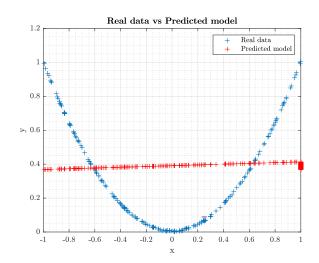


Fig. 9. Real data vs Predicted affine model.

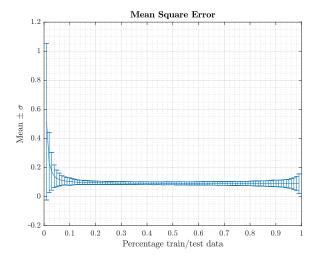


Fig. 10. $\,$ MSE for affine model as a function of the Training/test ratio.

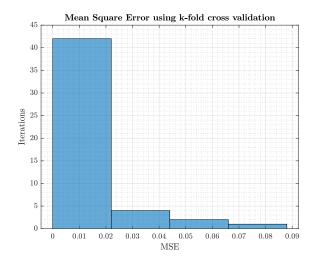


Fig. 11. Histogram for affine model using k-fold algorithm.

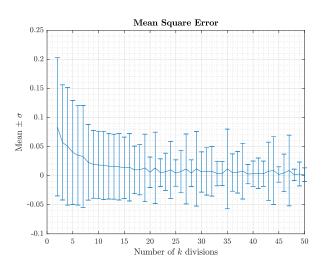


Fig. 12. MSE as a function of folds using k-fold algorithm.

V. Conclusions

This report shows different methods for predicting data using the linear regression method, along with the errors associated to it.

Comparing affine model and the linear one, it is clear how the error diminishes more rapidly in the latter. This is evidenced by comparing Figure 3 and Figure 10. The MSE when using the affine model is not only appreciably lower, but also much more defined, in the sense that the σ is very close to 0 between ratios of train/test data 0.3 to 0.6.

In both the affine and linear models, comparing Figures 5 and 6 fom the linear model and their analogous Figures for the affine model 11 and 12, it can be seen that the K-Fold algorithm is somewhat effective in reducing the MSE, as it is diminished with an increasing number of folds. This, however, does not apply to its standard deviation, which does not have an apparent correlation with the number of folds in either of the models.

In summary, with the different conclusions extracted from the aforementioned figures, along with the general result presented in Figures 1 and 9, it can be stated that the affine model better predicts the data generated by a quadratic curve with some randomized error. Futhermore, both models benefited from the use of the K-Fold Cros-Validation in its training.

References

- [1] Yale University. Linear Regression. 2021. URL: http://www.stat.yale.edu/Courses/1997-98/101/linreg.htm.
- [2] Machine Learning Glossary. Linear Regression. 2021. URL: https://ml-cheatsheet.readthedocs.io/en/latest/linear_regression.html#:~:text=Linear% 5C % 20Regression % 5C % 20is % 5C % 20a % 5C % 20supervised,Simple%5C%20regression.
- [3] Ian Goodfellow, Yoshua Bengio, and Aaron Courville. Deep learning. The MIT Press, 2017.

VI. Code

A. Figure 1

```
% Assignment 2: Linear Regression using Machine Learning
2
3 %-----
4
  % Date: 11/05/2021
   % Author/s:
6
   % Yi Qiang Ji
  % Biel Galiot
9
   % Gerar Villalta
10 % Oriol Miras
12 % Subject: Robotic Exploration of the Solar System
13 % Professor: Manel Soria & Arnau Miro
14
15 clc;
   close all;
16
17
   clear all;
18
  % Set interpreter to latex
19
  set(groot, 'defaultAxesTickLabelInterpreter', 'latex');
set(groot, 'defaulttextinterpreter', 'latex');
set(groot, 'defaultLegendInterpreter', 'latex');
21
22
23
24
   % Loop for every iteration
   iter = 1000;
26
   MSE = zeros(1, iter);
27
28
   for i=1:1:iter
29
30
      % Number of points
      nData = 200;
31
32
       % Generate data
33
      [xdata, ydata] = generateData(nData);
34
35
      % Split train and test data
36
      [Xtrain, Ytrain, Xtest, Ytest] = splitDataTrainAndTest(xdata, ydata, nData);
37
38
      % Compute coefficients
39
40
      w = computeW(Xtrain, Ytrain);
41
       % Predicted Y
42
      YtestPredicted = predictor(w, Xtest);
43
44
45
      % Minimum Squared Error
      MSE(i) = computeMSE(YtestPredicted, Ytest);
46
47
   % % Plots
48
   % figure(1)
49
  % plot(xdata,ydata,'+');
   % hold on
   % plot (Xtest, YtestPredicted, 'r+')
53
54
  end
55
   % plot_pdf = figure(1);
56
   % grid on;
   % grid minor;
58
   % box on;
59
   % xlabel('x');
   % ylabel('y');
   % title('\textbf{Real data vs Predicted model}');
   % legend('Real data', 'Predicted model');
63
64
   % % Save pdf
65
   % set(plot_pdf, 'Units', 'Centimeters');
% pos = get(plot_pdf, 'Position');
   % set(plot_pdf, 'PaperPositionMode', 'Auto', 'PaperUnits', 'Centimeters', ...
68
   % 'PaperSize', [pos(3), pos(4)]);
69
  % print(plot_pdf, 'data_vs_predicted.pdf', '-dpdf', '-r0')
70
72
   % print(gcf,'data_vs_predicted.png','-dpng','-r600');
73
74
75 plot_pdf2 = figure(2);
76
   histogram(MSE);
77 grid on;
   grid minor;
```

```
79 box on;
   xlabel('MSE');
81 ylabel('Iterations');
82 title('\textbf{Mean Square Error (TEST = 25\%)}');
83
   % % Save pdf
84
    % set(plot_pdf2, 'Units', 'Centimeters');
85
   % pos = get(plot_pdf2, 'Position');
86
    % set(plot_pdf2, 'PaperPositionMode', 'Auto', 'PaperUnits', 'Centimeters', ...
87
    % 'PaperSize',[pos(3), pos(4)]);
88
    % print(plot_pdf2, 'MSE_25_test.pdf', '-dpdf', '-r0')
90
   % % Save png
   % print(gcf,'MSE_25_test.png','-dpng','-r600');
92
93
94
   % Functions
95
    function [Xtrain, Ytrain, Xtest, Ytest] = splitDataTrainAndTest(xdata, ydata, nData)
       % Split data
97
       % Holdout validation percentage
98
       h_validation = 0.25; % Percentage
99
100
       train_data = round(h_validation*nData);
101
       % test_data = nData - train_data;
102
103
104
       Xtrain = xdata(1:train_data);
105
       Ytrain = ydata(1:train_data);
       Xtest = xdata((train_data+1):end);
106
107
       Ytest = ydata((train_data+1):end);
   end
108
109
110
    function [xdata, ydata] = generateData(nData)
111
       % Uniform distributed values between 'init' and 'final'
112
       % r = a + (b-a).*rand(N,1)
113
114
115
       % Initial and final range
       init = -1;
116
117
       final = 1;
118
119
       % Generate data
       xdata = -init + (init-(final))*rand(nData,1);
120
       ydata = xdata.^2 + 0.01*rand(nData,1); % Add some error
121
122
123
   function MSE = computeMSE(YtestPredicted, Ytest)
124
125
      MSE = immse(Ytest, YtestPredicted);
    end
127
    function w = computeW(Xtrain, Ytrain)
128
      w = (Xtrain.'*Xtrain)\(Xtrain.'*Ytrain);
129
130
132
    function y = predictor(w, x)
      y = w * x;
133
   end
134
135
136 function y = f(x)
137 \quad y = -x.^2;
   end
138
```

B. Figure 1.1

```
% Assignment 2: Linear Regression using Machine Learning
2
3
  % Date: 11/05/2021
  % Author/s:
  % Yi Qiang Ji
  % Biel Galiot
  % Gerar Villalta
9
10 % Oriol Miras
12 % Subject: Robotic Exploration of the Solar System
13 % Professor: Manel Soria & Arnau Miro
14
15 clc;
16 close all;
17 clear all;
```

```
18
   % Set interpreter to latex
19
20 set(groot, 'defaultAxesTickLabelInterpreter', 'latex');
21 set(groot,'defaulttextinterpreter','latex');
set (groot, 'defaultLegendInterpreter', 'latex');
23
25 % Loop for 1000 times
_{26} iter = 1000;
27
   % Loop for each percentage
   p_number = 100; % \( \Delta of increment \)
29
30 percentage = linspace(0.01,0.99,p_number); % From [0,1]
   MSE = zeros(p_number,iter);
31
32
33
   % Loop for every percentage
   for j = 1:1:length(percentage)
34
       for i=1:1:iter
36
37
          % Number of points
38
39
          nData = 200;
40
          % Generate data
41
          [xdata,ydata] = generateData(nData);
42
43
44
          % Split train and test data
          [Xtrain, Ytrain, Xtest, Ytest] = splitDataTrainAndTest(xdata, ydata, nData, percentage(j));
45
46
          % Compute coefficients
47
48
          w = computeW(Xtrain, Ytrain);
49
          % Predicted Y
50
          YtestPredicted = predictor(w, Xtest);
51
52
53
          % Minimum Squared Error
          MSE(j,i) = computeMSE(YtestPredicted, Ytest);
54
56
   % plot(xdata, ydata, '+');
57
58
   % hold on
   % plot(Xtest, YtestPredicted, 'r+')
59
61
       mean_MSE(1, j) = mean(MSE(j, :));
      std_MSE(1,j) = std(MSE(j,:));
62
   end
63
64
65 plot_pdf = figure(1);
   errorbar(percentage, mean_MSE(1,:), std_MSE(1,:));
66
   grid on;
67
68 grid minor:
69 box on;
70 xlabel('Percentage train/test data');
   ylabel('Mean $\pm$ $\sigma$');
71
   title('\textbf{Mean Square Error}');
72
73
74
   % % Save pdf
   % set(plot_pdf, 'Units', 'Centimeters');
76
    % pos = get(plot_pdf, 'Position');
    % set(plot_pdf, 'PaperPositionMode', 'Auto', 'PaperUnits', 'Centimeters', ...
77
   % 'PaperSize',[pos(3), pos(4)]);
% print(plot_pdf, 'MSE_error.pdf', '-dpdf', '-r0')
78
79
80
81
   % % Save png
   % print(gcf,'MSE_error.png','-dpng','-r600');
82
83
   % Functions
84
   function [Xtrain, Ytrain, Xtest, Ytest] = splitDataTrainAndTest(xdata, ydata, nData, percentage)
86
       % Split data
87
       % Holdout validation percentage
88
89
       h_validation = percentage; % Percentage
       train_data = round(h_validation*nData);
91
       % test_data = nData - train_data;
92
93
       Xtrain = xdata(1:train_data);
94
95
       Ytrain = ydata(1:train_data);
       Xtest = xdata((train_data+1):end);
96
97
       Ytest = ydata((train_data+1):end);
   end
98
99
   function [xdata, ydata] = generateData(nData)
100
```

```
% Uniform distributed values between 'init' and 'final'
102
103
        % r = a + (b-a).*rand(N,1)
104
        % Initial and final range
105
        init = -1;
106
        final = 1;
107
108
109
        % Generate data
       xdata = -init + (init-(final))*rand(nData,1);
ydata = xdata.^2 + 0.01*rand(nData,1); % Add some error
110
111
112
    end
113
    function MSE = computeMSE(YtestPredicted, Ytest)
114
       MSE = immse(Ytest, YtestPredicted);
115
116
117
118
    function w = computeW(Xtrain, Ytrain)
      w = (Xtrain.'*Xtrain)\(Xtrain.'*Ytrain);
119
120
121
122
    function y = predictor(w, x)
123
       y = w * x;
124
125
126
127 function y = f(x)
128
    y = -x.^2;
    end
```

C. Figure 2

```
2 clc;
3 close all;
4 clear all:
_{\rm 6} % Loop for 1000 times
7 iter = 1000;
9 % Loop for each nData
10 data = 10:5:500; % From [10,500]
11 MSE = zeros(length(data),iter);
13 % Loop for every nData
   for j = 1:1:length(data)
14
15
16
      for i=1:1:iter
17
         % Number of points
18
         nData = data(i);
19
20
21
         % Generate data
22
         [xdata, ydata] = generateData(nData);
23
          % Split train and test data
24
         [Xtrain, Ytrain, Xtest, Ytest] = splitDataTrainAndTest(xdata, ydata, nData);
25
26
27
         % Compute coefficients
         w = computeW(Xtrain, Ytrain);
29
         % Predicted Y
30
31
         YtestPredicted = predictor(w, Xtest);
32
         % Minimum Squared Error
33
         MSE(j,i) = computeMSE(YtestPredicted, Ytest);
34
35
36
37
      mean\_MSE(1,j) = mean(MSE(j,:));
      std_MSE(1,j) = std(MSE(j,:));
38
39
40
41 plot_pdf = figure(1);
42
   errorbar(data,mean_MSE(1,:),std_MSE(1,:));
43 grid on;
44 grid minor;
45 box on;
46 xlabel('nData');
   ylabel('Mean $\pm$ $\sigma$');
47
   title('\textbf{Mean Square Error}');
49
```

```
50 % % Save pdf
   % set(plot_pdf, 'Units', 'Centimeters');
   % pos = get(plot_pdf, 'Position');
   % set(plot_pdf, 'PaperPositionMode', 'Auto', 'PaperUnits', 'Centimeters', ...
53
   % 'PaperSize', [pos(3), pos(4)]);
54
   % print(plot_pdf, 'MSE_error_ndata_25.pdf', '-dpdf', '-r0')
   % % Save png
57
   % print(gcf,'MSE_error_ndata_25.png','-dpng','-r600');
58
59
   % Functions
   function [Xtrain, Ytrain, Xtest, Ytest] = splitDataTrainAndTest(xdata, ydata, nData)
61
       % Split data
63
       % Holdout validation percentage
64
      h_validation = 0.25; % Percentage
65
66
      train_data = round(h_validation*nData);
67
       % test_data = nData - train_data;
68
69
70
       Xtrain = xdata(1:train_data);
71
       Ytrain = ydata(1:train_data);
       Xtest = xdata((train_data+1):end);
72
       Ytest = ydata((train_data+1):end);
73
74
75
76
    function [xdata, ydata] = generateData(nData)
77
       % Initial and final range
78
      init = -1;
79
      final = 1;
80
81
82
       % Generate data
      xdata = -init + (init-(final))*rand(nData,1);
ydata = xdata.^2 + 0.01*rand(nData,1); % Add some error
83
84
85
   end
86
    function MSE = computeMSE(YtestPredicted, Ytest)
88
      MSE = immse(Ytest, YtestPredicted);
89
90
   function w = computeW(Xtrain, Ytrain)
91
     w = (Xtrain.'*Xtrain)\(Xtrain.'*Ytrain);
93
94
   function y = predictor(w,x)
95
96
     y = w * x;
97
   end
98
99
   function y = f(x)
100
y = -x.^2;
102 end
```

D. Figure 3

```
2
   % Assignment 2: Linear Regression using Machine Learning
4
5 % Date: 11/05/2021
  % Author/s:
7 % Yi Qiang Ji
   % Biel Galiot
   % Gerar Villalta
9
10 % Oriol Miras
12 % Subject: Robotic Exploration of the Solar System
13 % Professor: Manel Soria & Arnau Miro
14
15 clc;
16 close all;
17
   clear all;
18
19 % Set interpreter to latex
set(groot,'defaultAxesTickLabelInterpreter','latex');
set(groot,'defaulttextinterpreter','latex');
22
   set(groot, 'defaultLegendInterpreter', 'latex');
23
24
```

```
25
   % Divisions
    k_{div} = 2:1:50;
    % MSE vector
28
29
   MSE = zeros(1,length(k_div));
   % Number of points
31
   nData = 200;
32
33
34
    % Generate data
    [xdata,ydata] = generateData(nData);
35
36
37
    for j=1:1:length(k_div)
38
        % Loop for every division
39
       for i=1:1:k_div(j)
40
41
           MSE\_div = zeros(k\_div(j),1);
42
           % Split train and test data
43
           [Xtrain, Ytrain, Xtest, Ytest] = splitDataTrainAndTest(xdata, ydata, nData, i, k_div(j));
44
45
          % Compute coefficients
46
47
          w = computeW(Xtrain, Ytrain);
48
           % Predicted Y
49
50
          YtestPredicted = predictor(w, Xtest);
51
           % Minimum Squared Error
52
          MSE_div(i,:) = computeMSE(YtestPredicted, Ytest);
53
       % % Plots
54
55
       % figure(1)
56
       % plot(xdata, ydata, '+');
       % hold on
57
       % plot(Xtest, YtestPredicted, 'r+')
58
59
       end
          MSE(1,j) = mean(MSE_div);
mean_MSE = MSE;
60
61
           std_MSE(1,j) = std(MSE_div);
63
           hold on:
   end
64
65
   plot_pdf = figure(1);
66
67 histogram(MSE, 10);
   grid on;
68
   grid minor;
69
70 box on;
71
   xlabel('MSE');
   ylabel('Iterations');
   title('\textbf{Mean Square Error using k-fold cross validation}');
73
74
    % % Save pdf
75
    % set(plot_pdf, 'Units', 'Centimeters');
% pos = get(plot_pdf, 'Position');
76
    % set(plot_pdf, 'PaperPositionMode', 'Auto', 'PaperUnits', 'Centimeters', ...
78
    % 'PaperSize', [pos(3), pos(4)]);
79
    % print(plot_pdf, 'MSE_kfold.pdf', '-dpdf', '-r0')
80
81
   % % Save png
83
    % print(gcf,'MSE_kfold.png','-dpng','-r600');
84
   plot_pdf2 = figure(2);
85
    \texttt{errorbar(k\_div,mean\_MSE(1,:),std\_MSE(1,:));}
86
    grid on;
87
88
    grid minor;
   box on;
89
   xlabel('Number of $k$ divisions');
ylabel('Mean $\pm$ $\sigma$');
90
91
   title('\textbf{Mean Square Error}');
92
93
    % % Save pdf
94
    % set(plot_pdf2, 'Units', 'Centimeters');
% pos = get(plot_pdf2, 'Position');
95
96
    % set(plot_pdf2, 'PaperPositionMode', 'Auto', 'PaperUnits', 'Centimeters', ...
    % 'PaperSize', [pos(3), pos(4)]);
98
    % print(plot_pdf2, 'MSE_kfold_error.pdf', '-dpdf', '-r0')
100
   % % Save png
101
   % print(gcf,'MSE_kfold_error.png','-dpng','-r600');
102
103
    % Functions
104
    function [Xtrain,Ytrain,Xtest,Ytest] = splitDataTrainAndTest(xdata,ydata,nData, index, k_div)
105
106
107
       % Split data
       % Holdout validation percentage
```

```
% h_validation = 0.25; % Percentage
109
110
       % train_data = round(h_validation*nData);
111
       % test_data = nData - train_data;
112
113
114
       div = floor(nData/k_div);
115
       Xtest = xdata(((index-1)*div + 1):index*div);
       Ytest = ydata(((index-1)*div + 1):index*div);
116
       Xtrain = setdiff(xdata, Xtest);
117
       Ytrain = setdiff(ydata, Ytest);
118
119
   end
120
    function [xdata,ydata] = generateData(nData)
122
       % Uniform distributed values between 'init' and 'final'
123
124
       % r = a + (b-a).*rand(N,1)
125
       % Initial and final range
126
       init = -1;
127
       final = 1;
128
129
130
       % Generate data
       xdata = -init + (init-(final))*rand(nData,1);
131
       ydata = xdata.^2 + 0.01*rand(nData,1); % Add some error
132
133
134
135
    function MSE = computeMSE(YtestPredicted, Ytest)
      MSE = immse(Ytest, YtestPredicted);
136
137
138
139
   function w = computeW(Xtrain, Ytrain)
140
      w = (Xtrain.'*Xtrain)\(Xtrain.'*Ytrain);
141
142
    function y = predictor(w, x)
143
144
      y = w * x;
145
    end
146
147
   function y = f(x)
148
149 \quad y = -x.^2;
150
   end
```

E. Figure 4

```
2 % Assignment 2: Linear Regression using Machine Learning
  % Date: 11/05/2021
5
  % Author/s:
6
  % Yi Qiang Ji
   % Biel Galiot
  % Gerar Villalta
10 % Oriol Miras
11
12 % Subject: Robotic Exploration of the Solar System
13
  % Professor: Manel Soria & Arnau Miro
15 clc;
16 close all:
17 clear all;
  % Set interpreter to latex
19
  set(groot, 'defaultAxesTickLabelInterpreter', 'latex');
20
  set(groot, 'defaulttextinterpreter', 'latex');
21
22 set(groot, 'defaultLegendInterpreter', 'latex');
23
25
   % Divisions
26 k_div = 4;
27
28 % MSE_vector
29 MSE = zeros(1,length(k_div));
30
31 % Number of points
nData = 10:5:500; % From [10,500]
33
35
  for j=1:1:length(nData)
```

```
36
       % Generate data
37
       [xdata, ydata] = generateData(nData(j));
38
39
       % Loop for every division
40
41
       for i=1:1:k_div
42
          MSE\_div = zeros(k\_div, 1);
43
44
45
          % Split train and test data
          [Xtrain, Ytrain, Xtest, Ytest] = splitDataTrainAndTest(xdata, ydata, nData(j), i, k_div);
46
47
          % Compute coefficients
 48
          w = computeW(Xtrain, Ytrain);
49
50
          % Predicted Y
51
          YtestPredicted = predictor(w, Xtest);
52
53
          % Minimum Squared Error
54
         MSE_div(i,:) = computeMSE(YtestPredicted, Ytest);
55
       % % Plots
56
57
       % figure(1)
58
       % plot(xdata, ydata, '+');
       % hold on
59
       % plot(Xtest, YtestPredicted, 'r+')
60
61
       end
62
          MSE(1,j) = mean(MSE_div);
          mean_MSE = MSE;
63
          std_MSE(1, j) = std(MSE_div);
64
          hold on;
65
66 end
67
68 plot_pdf = figure(1);
69 histogram (MSE, 10);
70 grid on;
71
   grid minor:
72 box on;
73 xlabel('MSE');
   ylabel('Iterations');
75 title('\textbf{Mean Square Error using k-fold cross validation as a function of nData}');
76
77
   % % Save pdf
   % set(plot_pdf, 'Units', 'Centimeters');
    % pos = get(plot_pdf, 'Position');
79
    % set(plot_pdf, 'PaperPositionMode', 'Auto', 'PaperUnits', 'Centimeters', ...
80
    % 'PaperSize', [pos(3), pos(4)]);
81
    % print(plot_pdf, 'MSE_kfold_nData.pdf', '-dpdf', '-r0')
82
    % % Save png
84
   % print(gcf,'MSE_kfold_nData.png','-dpng','-r600');
85
86
87 plot_pdf2 = figure(2);
 88 errorbar(nData, mean_MSE(1,:), std_MSE(1,:));
89 grid on;
90 grid minor;
91 box on:
92 xlabel('nData');
93 ylabel('Mean $\pm$ $\sigma$');
94
   title('\textbf{Mean Square Error}');
95
    % % Save pdf
96
   % set(plot_pdf2, 'Units', 'Centimeters');
97
   % pos = get(plot_pdf2, 'Position');
    % set(plot_pdf2, 'PaperPositionMode', 'Auto', 'PaperUnits', 'Centimeters', ...
    % 'PaperSize', [pos(3), pos(4)]);
100
    % print(plot_pdf2, 'MSE_kfold_nData_error.pdf', '-dpdf', '-r0')
101
102
   % % Save png
103
   % print(gcf,'MSE_kfold_nData_error.png','-dpng','-r600');
104
105
106
    % Functions
    function [Xtrain,Ytrain,Xtest,Ytest] = splitDataTrainAndTest(xdata,ydata,nData, index, k_div)
107
108
       % Split data
109
       % Holdout validation percentage
110
       % h_validation = 0.25; % Percentage
111
112
113
       % train_data = round(h_validation*nData);
       % test_data = nData - train_data;
114
115
       div = floor(nData/k div);
116
       Xtest = xdata(((index-1)*div + 1):index*div);
117
       Ytest = ydata(((index-1)*div + 1):index*div);
118
       Xtrain = setdiff(xdata, Xtest);
```

```
Ytrain = setdiff(ydata, Ytest);
120
121
    end
122
    function [xdata, ydata] = generateData(nData)
123
124
        \mbox{\ensuremath{\mbox{\$}}} Uniform distributed values between 'init' and 'final'
125
126
        % r = a + (b-a).*rand(N,1)
127
        % Initial and final range
128
       init = -1;
129
       final = 1;
130
131
        % Generate data
       xdata = -init + (init-(final))*rand(nData,1);
ydata = xdata.^2 + 0.01*rand(nData,1); % Add some error
133
134
   end
135
136
     function MSE = computeMSE(YtestPredicted, Ytest)
137
       MSE = immse(Ytest, YtestPredicted);
138
139
140
141
     function w = computeW(Xtrain, Ytrain)
      w = (Xtrain.'*Xtrain)\(Xtrain.'*Ytrain);
142
143
144
145
    function y = predictor(w,x)
146
      y = w * x;
147
148
149
150 function y = f(x)
y = -x.^2;
   end
```

F. Extra 1

```
% Assignment 2: Linear Regression using Machine Learning
3
4
5 % Date: 11/05/2021
  % Author/s:
  % Yi Qiang Ji
  % Biel Galiot
   % Gerar Villalta
9
10 % Oriol Miras
12 % Subject: Robotic Exploration of the Solar System
13 % Professor: Manel Soria & Arnau Miro
14
15 clc;
16 close all;
17
   clear all;
18
   % Set interpreter to latex
19
o set (groot, 'defaultAxesTickLabelInterpreter', 'latex');
set (groot, 'defaulttextinterpreter', 'latex');
set (groot, 'defaultLegendInterpreter', 'latex');
24
  % Loop for 1000 times
25
_{26} iter = 1000;
28 % Loop for each percentage
29 p_number = 100; % Δof increment
  percentage = linspace(0.01,0.99,p_number); % From [0,1]
30
31 MSE = zeros(p_number,iter);
   % Loop for every percentage
   for j = 1:1:length(percentage)
34
35
       for i=1:1:iter
36
37
          % Number of points
38
          nData = 200;
39
40
          % Generate data
41
42
          [xdata, ydata] = generateData(nData);
43
44
          % Split train and test data
```

```
45
          [Xtrain, Ytrain, Xtest, Ytest] = splitDataTrainAndTest(xdata, ydata, nData, percentage(j));
 46
47
          % Compute coefficients
          w = computeW(Xtrain, Ytrain);
48
49
50
          % Predicted Y
          YtestPredicted = predictor(w, Xtest);
51
52
          % Minimum Squared Error
53
          MSE(j,i) = computeMSE(YtestPredicted, Ytest);
54
55
56
          % Plots
   % plot(xdata,ydata,'+');
    % hold on
58
   % plot(Xtest, YtestPredicted, 'r+')
59
60
       end
61
       mean_MSE(1,j) = mean(MSE(j,:));
       std_MSE(1,j) = std(MSE(j,:));
   end
63
64
65 plot_pdf = figure(1);
    errorbar(percentage, mean_MSE(1,:), std_MSE(1,:));
66
67 grid on:
68 grid minor;
69 box on;
70 xlabel('Percentage train/test data');
    ylabel('Mean $\pm$ $\sigma$');
71
   title('\textbf{Mean Square Error}');
73
   % % Save pdf
74
   % set(plot_pdf, 'Units', 'Centimeters');
% pos = get(plot_pdf, 'Position');
75
76
    % set(plot_pdf, 'PaperPositionMode', 'Auto', 'PaperUnits', 'Centimeters', ...
    % 'PaperSize', [pos(3), pos(4)]);
78
    % print(plot_pdf, 'MSE_afi.pdf', '-dpdf', '-r0')
79
80
   % % Save png
81
   % print(gcf,'MSE_afi.png','-dpng','-r600');
83
   % Functions
84
   function [Xtrain, Ytrain, Xtest, Ytest] = splitDataTrainAndTest(xdata, ydata, nData, percentage)
85
86
       % Split data
       % Holdout validation percentage
88
      h_validation = percentage; % Percentage
89
90
91
      train_data = round(h_validation*nData);
       % test_data = nData - train_data;
93
       Xtrain = xdata(1:train_data);
94
       Xtrain = [xdata(1:train_data) ones(size(Xtrain,1),1)];
95
96
       Ytrain = ydata(1:train_data);
97
98
       Xtest = xdata((train_data+1):end);
       Xtest = [xdata((train_data+1):end) ones(size(Xtest,1),1)];
99
100
       Ytest = ydata((train_data+1):end);
101
    end
103
    function [xdata,ydata] = generateData(nData)
104
       % Uniform distributed values between 'init' and 'final'
105
106
       % r = a + (b-a).*rand(N,1)
107
       % Initial and final range
108
      init = -1;
109
       final = 1;
110
111
112
       % Generate data
       xdata = -init + (init-(final))*rand(nData,1);
113
       ydata = xdata.^2 + 0.01*rand(nData,1); % Add some error
114
   end
115
116
    function MSE = computeMSE(YtestPredicted, Ytest)
117
      MSE = immse(Ytest, YtestPredicted);
118
119
120
    function w = computeW(Xtrain, Ytrain)
121
122
      w = (Xtrain.'*Xtrain)\(Xtrain.'*Ytrain);
123
124
    function y = predictor(w, x)
125
      y = x * w;
126
127
    end
```

```
129

130 function y = f(x)

131 y = -x.^2;

132 end
```

G. Extra 2

```
% Assignment 2: Linear Regression using Machine Learning
3
  % Date: 11/05/2021
   % Author/s:
6
   % Yi Qiang Ji
   % Biel Galiot
   % Gerar Villalta
9
10 % Oriol Miras
12 % Subject: Robotic Exploration of the Solar System
13 % Professor: Manel Soria & Arnau Miro
14
15 clc;
  close all;
16
  clear all;
17
18
19
  % Set interpreter to latex
  set(groot, 'defaultAxesTickLabelInterpreter', 'latex');
  set(groot, 'defaulttextinterpreter', 'latex');
set(groot, 'defaultLegendInterpreter', 'latex');
21
22
23
24
25
   % Divisions
26
   k_{div} = 2:1:50;
   % MSE vector
28
MSE = zeros(1, length(k_div));
   % Number of points
31
  nData = 200;
32
33
   % Generate data
34
35
   [xdata, ydata] = generateData(nData);
36
37
   for j=1:1:length(k_div)
38
       % Loop for every division
39
40
      for i=1:1:k_div(j)
41
          MSE\_div = zeros(k\_div(j),1);
42
          % Split train and test data
43
          [Xtrain, Ytrain, Xtest, Ytest] = splitDataTrainAndTest(xdata, ydata, nData, i, k_div(j));
44
45
          % Compute coefficients
46
          w = computeW(Xtrain, Ytrain);
47
48
          % Predicted Y
49
50
         YtestPredicted = predictor(w, Xtest);
51
          % Minimum Squared Error
         MSE_div(i,:) = computeMSE(YtestPredicted, Ytest);
53
      % % Plots
54
      % figure(1)
55
56
      % plot(xdata,ydata,'+');
      % hold on
57
       % plot(Xtest, YtestPredicted, 'r+')
58
59
      end
         MSE(1, j) = mean(MSE_div);
mean_MSE = MSE;
60
61
          std_MSE(1,j) = std(MSE_div);
63
          hold on;
64 end
65
66 plot_pdf = figure(1);
67 histogram (MSE);
68 grid on;
69 grid minor;
70 box on;
71
  xlabel('MSE');
  ylabel('Iterations');
   title('\textbf{Mean Square Error using k-fold cross validation}');
```

```
74
    % % Save pdf
75
   % set(plot_pdf, 'Units', 'Centimeters');
    % pos = get(plot_pdf, 'Position');
77
    % set(plot_pdf, 'PaperPositionMode', 'Auto', 'PaperUnits', 'Centimeters', ...
78
   % 'PaperSize', [pos(3), pos(4)]);
79
    % print(plot_pdf, 'MSE_afi_kfold.pdf', '-dpdf', '-r0')
80
81
   % % Save png
82
   % print(gcf,'MSE_afi_kfold.png','-dpng','-r600');
83
85 plot_pdf2 = figure(2);
   errorbar(k_div,mean_MSE(1,:),std_MSE(1,:));
   grid on;
87
88
   grid minor:
89
   box on;
   xlabel('Number of $k$ divisions');
90
   ylabel('Mean $\pm$ $\sigma$');
   title('\textbf{Mean Square Error}');
92
93
94
   % % Save pdf
    % set(plot_pdf2, 'Units', 'Centimeters');
95
    % pos = get(plot_pdf2, 'Position');
    % set(plot_pdf2, 'PaperPositionMode', 'Auto', 'PaperUnits', 'Centimeters', ...
97
    % 'PaperSize',[pos(3), pos(4)]);
98
99
    % print(plot_pdf2, 'MSE_afi_kfold_error.pdf', '-dpdf', '-r0')
100
   % % Save png
101
    % print(gcf, 'MSE_afi_kfold_error.png', '-dpng', '-r600');
102
103
104
    % Functions
105
    function [Xtrain, Ytrain, Xtest, Ytest] = splitDataTrainAndTest(xdata, ydata, nData, index, k_div)
106
       % Split data
107
       % Holdout validation percentage
108
109
       % h_validation = 0.25; % Percentage
110
       % train_data = round(h_validation*nData);
112
       % test_data = nData - train_data;
113
       div = floor(nData/k_div);
114
       Xtest = xdata(((index-1)*div + 1):index*div);
115
       Xtest = [xdata(((index-1)*div + 1):index*div) ones(size(Xtest,1),1)];
117
       Ytest = ydata(((index-1)*div + 1):index*div);
118
       Xtrain = setdiff(xdata, Xtest);
119
       Xtrain = [setdiff(xdata, Xtest) ones(size(Xtrain, 1), 1)];
120
121
       Ytrain = setdiff(ydata, Ytest);
122
123
    function [xdata, ydata] = generateData(nData)
124
125
       % Uniform distributed values between 'init' and 'final'
126
127
       % r = a + (b-a).*rand(N,1)
128
       \mbox{\ensuremath{\upsigma}} Initial and final range
129
130
       init = -1;
       final = 1;
131
132
       % Generate data
133
       xdata = -init + (init-(final))*rand(nData,1);
ydata = xdata.^2 + 0.01*rand(nData,1); % Add some error
134
135
136
    end
137
    function MSE = computeMSE(YtestPredicted, Ytest)
138
      MSE = immse(Ytest, YtestPredicted);
139
140
141
    function w = computeW(Xtrain, Ytrain)
142
      w = (Xtrain.'*Xtrain)\(Xtrain.'*Ytrain);
143
144
145
    function y = predictor(w, x)
146
147
       y = x * w;
148
149
150
151 function y = f(x)
_{152} y = -x.^2;
  end
153
```