EE2211 Tutorial 7

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Q1

This question explores the use of Pearson's correlation as a feature selection metric. We are given the following training dataset:

	Datapoint 1	Datapoint 2	Datapoint 3	Datapoint 4	Datapoint 5
Feature 1	0.3510	2.1812	0.2415	-0.1096	0.1544
Feature 2	1.1796	2.1068	1.7753	1.2747	2.0851
Feature 3	-0.9852	1.3766	-1.3244	-0.6316	-0.8320
Target y	0.2758	1.4392	-0.4611	0.6154	1.0006

What are the top two features we should select if we use Pearson's correlation as a feature selection metric?

Q1

Given N pairs of datapoints $\{(a_1, b_1), (a_2, b_2), \cdots, (a_N, b_N)\}$, the Pearson's correlation r is defined as

$$r = \frac{Cov(a, b)}{\sigma_a \sigma_b}$$

where

$$\sigma_a = \sqrt{\frac{1}{N}\sum_{n=1}^{N}(a_i - \bar{a})^2} \qquad \sigma_b = \sqrt{\frac{1}{N}\sum_{n=1}^{N}\left(b_i - \bar{b}\right)^2}$$

Empirical standard deviation of a and b

and

$$Cov(a, b) = \frac{1}{N}\sum_{n=1}^{N}(a_i - \bar{a})\left(b_i - \bar{b}\right)$$

Empirical covariance between a and b

where

$$\bar{a} = \sum_{n=1}^{N} a_n \qquad \bar{b} = \sum_{n=1}^{N} b_n$$

Empirical means of a and b respectively

Q1

The Pearson correlation coefficient (often called Pearson's r) is a statistical measure that quantifies the linear relationship between two continuous variables. It is one of the most widely used correlation measures in statistics and is often used to determine whether an increase in one variable tends to be associated with an increase or decrease in another variable.

Key Characteristics:

Range: The Pearson correlation coefficient ranges from -1 to 1.

- +1: Indicates a perfect positive linear relationship. As one variable increases, the other increases proportionally.
- -1: Indicates a perfect negative linear relationship. As one variable increases, the other decreases proportionally.
- 0: Indicates no linear relationship between the variables. However, they may still have a non-linear relationship.

Q1

Pearson's correlation $r = \frac{Cov(a,b)}{\sigma_a \sigma_b}$

$$\text{Mean of Feature 1} = \mu_1 = \frac{0.3510+2.1812+0.2415-0.1096+0.1544}{5} = 0.5637$$

$$\text{Mean of Feature 2} = \mu_2 = \frac{1.1796+2.1068+1.7753+1.2747+2.0851}{5} = 1.6843$$

$$\text{Mean of Feature 3} = \mu_3 = \frac{-0.9852+1.3766-1.3244-0.6316-0.8320}{5} = -0.4793$$

$$\text{Mean of Target y} = \mu_y = \frac{0.2758+1.4392-0.4611+0.6154+1.0006}{5} = 0.5740$$

$$\text{Feature 1 std} = \sigma_1 = \sqrt{\frac{(0.3510-\mu_1)^2+(2.1812-\mu_1)^2+(0.2415-\mu_1)^2+(-0.1096-\mu_1)^2+(0.1544-\mu_1)^2}{5}} = 0.8229$$

$$\text{Feature 2 std} = \sigma_2 = \sqrt{\frac{(1.1796-\mu_2)^2+(2.1068-\mu_2)^2+(1.7753-\mu_2)^2+(1.2747-\mu_2)^2+(2.0851-\mu_2)^2}{5}} = 0.3924$$

$$\text{Feature 3 std} = \sigma_3 = \sqrt{\frac{(-0.9852-\mu_3)^2+(1.3766-\mu_3)^2+(-1.3244-\mu_3)^2+(-0.6316-\mu_3)^2+(-0.8320-\mu_3)^2}{5}} = 0.9552$$

$$\text{Target y std} = \sigma_y = \sqrt{\frac{(0.2758-\mu_y)^2+(1.4392-\mu_y)^2+(-0.4611-\mu_y)^2+(0.6154-\mu_y)^2+(1.0006-\mu_y)^2}{5}} = 0.6469$$

Q1

- Pearson's correlation $r = \frac{Cov(a,b)}{\sigma_a \sigma_b}$

$$\text{Cov(Feature 1, y)} = \frac{1}{5}[(0.3510 - \mu_1)(0.2758 - \mu_y) + (2.1812 - \mu_1)(1.4392 - \mu_y) + (0.2415 - \mu_1)(-0.4611 - \mu_y) + (-0.1096 - \mu_1)(0.6154 - \mu_y) + (0.1544 - \mu_1)(1.0006 - \mu_y)] = 0.3188$$

$$\text{Cov(Feature 2,y)} = \frac{1}{5}[(1.1796 - \mu_2)(0.2758 - \mu_y) + (2.1068 - \mu_2)(1.4392 - \mu_y) + (1.7753 - \mu_2)(-0.4611 - \mu_y) + (1.2747 - \mu_2)(0.6154 - \mu_y) + (2.0851 - \mu_2)(1.0006 - \mu_y)] = 0.1152$$

$$\text{Cov(Feature 3,y)} = \frac{1}{5}[(-0.9852 - \mu_3)(0.2758 - \mu_y) + (1.3766 - \mu_3)(1.4392 - \mu_y) + (-1.3244 - \mu_3)(-0.4611 - \mu_y) + (-0.6316 - \mu_3)(0.6154 - \mu_y) + (-0.8320 - \mu_3)(1.0006 - \mu_y)] = 0.4949$$

$$\text{Correlation of Feature 1 \& y} = \frac{Cov(Feature\ 1,y)}{\sigma_1 \sigma_y} = \frac{0.3188}{0.8229 \times 0.6469} = \boxed{0.5988}$$

$$\text{Correlation of Feature 2 \& y} = \frac{Cov(Feature\ 2,y)}{\sigma_2 \sigma_y} = \frac{0.1152}{0.3924 \times 0.6469} = 0.4537$$

$$\text{Correlation of Feature 3 \& y} = \frac{Cov(Feature\ 3,y)}{\sigma_3 \sigma_y} = \frac{0.4949}{0.9552 \times 0.6469} = \boxed{0.8009}$$

Therefore, the top 2 features are Feature 1 and Feature 3.

Q1

```python
import numpy as np

data = np.array([[0.3510,   2.1812,     0.2415,     -0.1096,     0.1544],
                 [1.1796,   2.1068,     1.7753,     1.2747,      2.0851],
                 [-0.9852,  1.3766,     -1.3244,    -0.6316,     -0.8320]])

target = np.array([0.2758, 1.4392, -0.4611, 0.6154, 1.0006])

from scipy.stats import pearsonr
for i in range(len(data)):
    r, _ = pearsonr(data[i], target)

    print("Pearson\'s r of Feature", i+1, "and y=", r)
```

Q2

This question further explores linear regression and ridge regression. The following data pairs are used for training and testing:

Training:

$$\{x = -10\} \rightarrow \{y = 4.18\}$$
$$\{x = -8\} \rightarrow \{y = 2.42\}$$
$$\{x = -3\} \rightarrow \{y = 0.22\}$$
$$\{x = -1\} \rightarrow \{y = 0.12\}$$
$$\{x = 2\} \rightarrow \{y = 0.25\}$$
$$\{x = 7\} \rightarrow \{y = 3.09\}$$

Testing:

$$\{x = -9\} \rightarrow \{y = 3\}$$
$$\{x = -7\} \rightarrow \{y = 1.81\}$$
$$\{x = -5\} \rightarrow \{y = 0.80\}$$
$$\{x = -4\} \rightarrow \{y = 0.25\}$$
$$\{x = -2\} \rightarrow \{y = -0.19\}$$
$$\{x = 1\} \rightarrow \{y = 0.4\}$$
$$\{x = 4\} \rightarrow \{y = 1.24\}$$
$$\{x = 5\} \rightarrow \{y = 1.68\}$$
$$\{x = 6\} \rightarrow \{y = 2.32\}$$
$$\{x = 9\} \rightarrow \{y = 5.05\}$$

Q2

This question further explores linear regression and ridge regression. The following data pairs are used for training and testing:

a) Use the polynomial model from orders 1 to 6 to train and test the data without regularization. Plot the Mean Squared Errors (MSE) over orders from 1 to 6 for both the training and the test sets. Which model order provides the best MSE in the training and test sets? Why?

b) Use regularization (ridge regression) $\lambda = 1$ for all orders and repeat the same analyses. Compare the plots of (a) and (b). What do you see?

Main Function: Tut_Q2

Data Generation

- Training Data: Input features (x) and labels (y) for training the model.
- Test Data: Input features (xt) and labels (yt) for testing the model.

↓

Regressor Creation

CreateRegressors(): A function that generates regressor matrices based on the input features and the maximum polynomial order.

↓

Model Training

EstimateRegressionCoefficients(): A function that estimates the coefficients of the regression model, with an option for regularization.

↓

Model Prediction

PerformPrediction(): A function that uses the estimated coefficients and regressor matrices to make predictions.

↓

Performance Evaluation

Mean Squared Error (MSE): Calculation of MSE for both training and test sets to evaluate the model's performance.

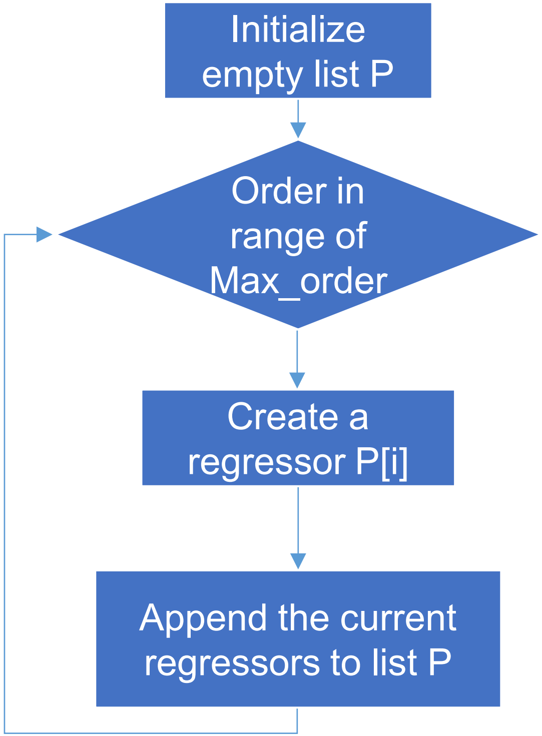
↓

Visualization

Plotting of Predicted Curves: Using matplotlib to plot the actual and predicted values.
Plotting of MSE: Visual representation of the MSE for different polynomial orders.

Function: CreateRegressors()

```
def CreateRegressors(x, max_order):

    # x is assumed to be array of length N
    # return P = list of regressors based on max_order
    # P[i] are regressors for order i+1 and is of size N x (order+1), where
    # N is number of data points

    P = [] #initialize empty list
    for order in range(1, max_order+1):
        current_regressors = np.zeros([len(x), order+1])
        current_regressors[:,0] = np.ones(len(x))
        for i in range(1, order+1):
            current_regressors[:,i] = np.power(x, i)
        P.append(current_regressors)

    return P
```

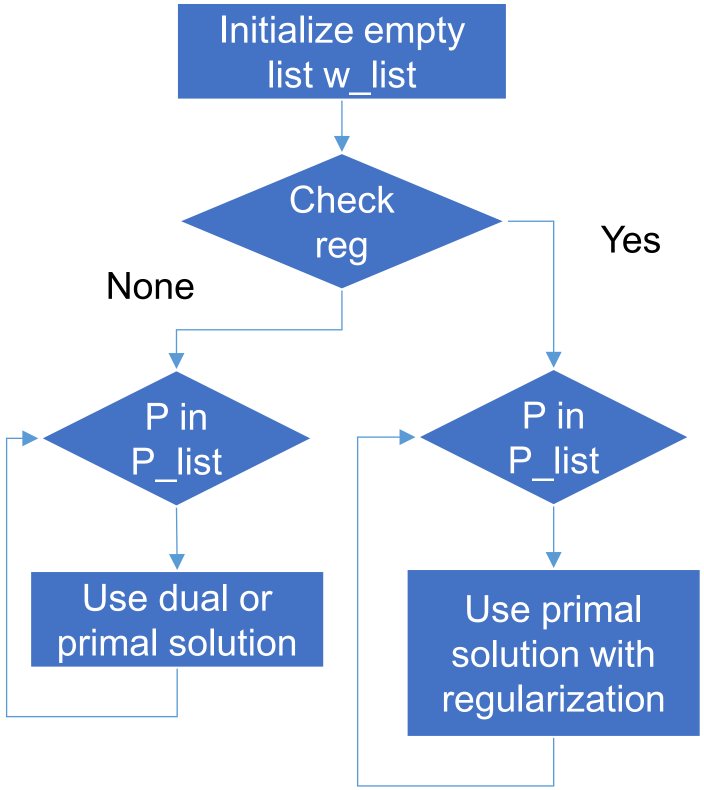


Create a regressor P[i]

- Set the first column of the matrix to ones. This represents the constant term in the polynomial.
- Set column i to x to the power of i: Calculate the power of x raised to the current index i and set it as the value for the current column in the matrix.

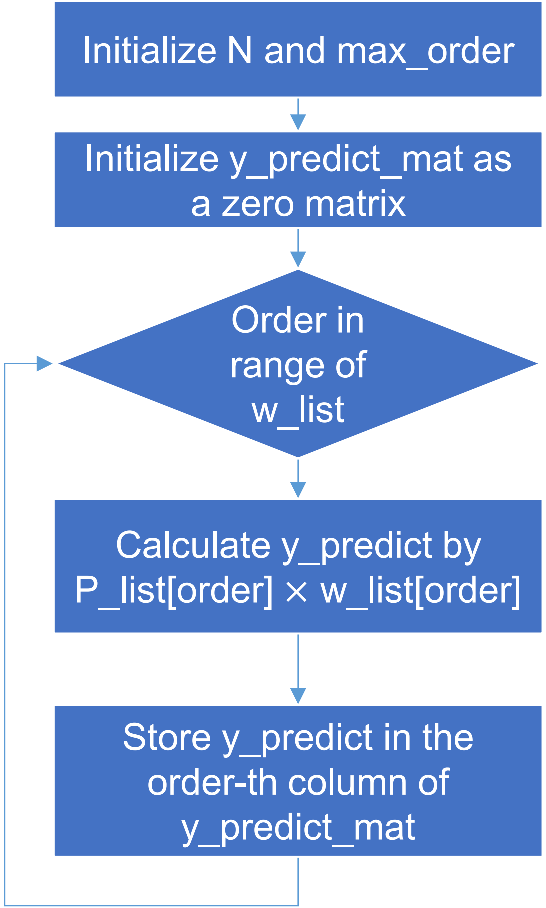
Function: `EstimateRegressionCoefficients()`

```
def EstimateRegressionCoefficients(P_list, y, reg=None):

    # P_list is a list
    # P_list[i] are regressors for order i+1 and is of size N x
(order+1), where
    # N is number of data points

    w_list = []
    if reg is None:

        for P in P_list:
            if(P.shape[1] > P.shape[0]): #use dual solution
                w = P.T @ inv(P @ P.T) @ y
            else: # use primal solution
                w = (inv(P.T @ P) @ P.T) @ y
            w_list.append(w)
    else:

        for P in P_list:
            w = (inv(P.T @ P + reg*np.eye(P.shape[1]) ) @ P.T) @ y
            w_list.append(w)

    return w_list
```



Function: `PerformPrediction()`

```
def PerformPrediction(P_list, w_list):

    # P_list is list of regressors
    # w_list is list of coefficients
    # Output is y_predict_mat which N x max_order, where N is
the number of samples

    N = P_list[0].shape[0]
    max_order = len(P_list)
    y_predict_mat = np.zeros([N, max_order])
    for order in range(len(w_list)):
        y_predict = np.matmul(P_list[order], w_list[order])
        y_predict_mat[:,order] = y_predict

    return y_predict_mat
```



Q2

This question further explores linear regression and ridge regression. The following data pairs are used for training and testing:

a) Use the polynomial model from orders 1 to 6 to train and test the data without regularization. Plot the Mean Squared Errors (MSE) over orders from 1 to 6 for both the training and the test sets. Which model order provides the best MSE in the training and test sets? Why?

Q2(a)

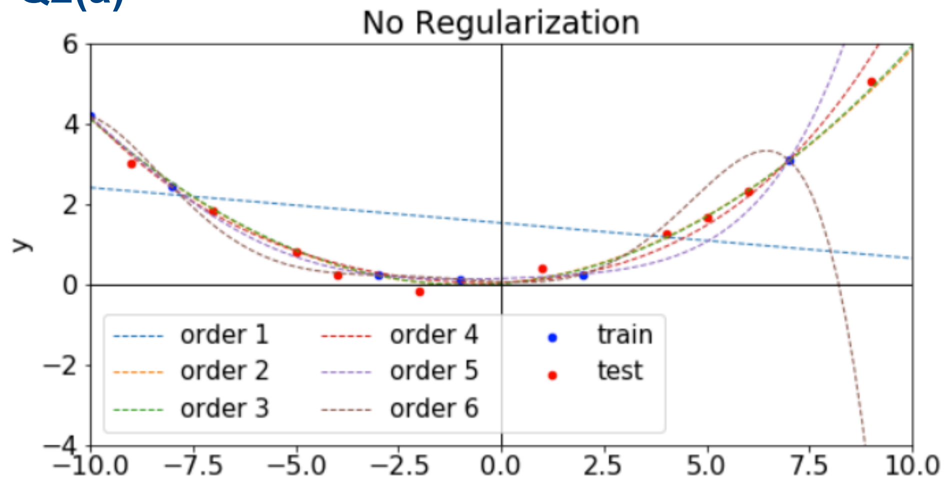
There are 6 training data points.

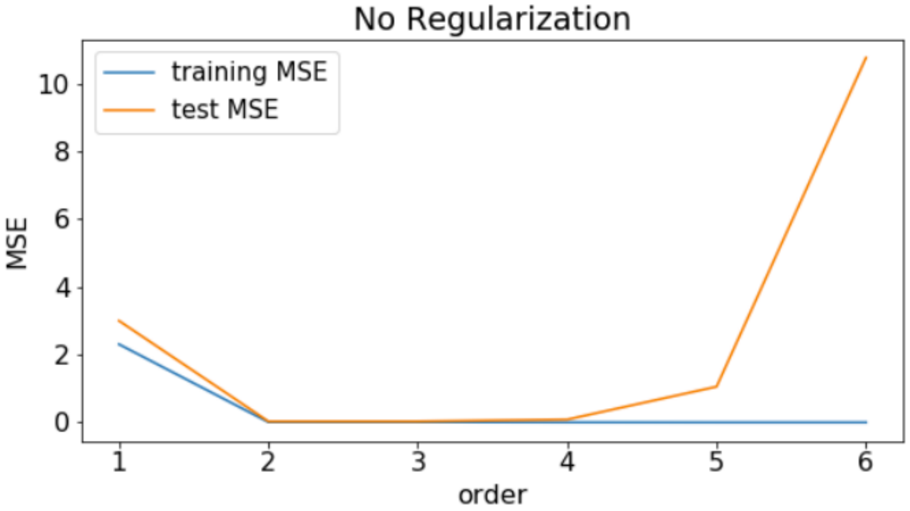
- For polynomial orders 1 to 5, we can use the Primal solution: $\hat{w} = (P^T P)^{-1} P^T y$
- For order 6, there are 7 unknowns, so the system is under-determined, so we use the Dual solution: $\hat{w} = P^T (P P^T)^{-1} y$

====== No Regularization =======

Training MSE:	[2.3071.	8.4408e-03	8.3026e-03	1.7348e-03	3.8606e-25	2.3656e-17]
Test MSE:	[3.0006	0.0296	0.0301	0.0854	1.0548	10.7674]

Q2(a)





Observe that the estimated polynomial curves for orders 5 and 6 pass through the training samples exactly. This results in training MSE of virtually 0, but high test MSE => overfitting

Note that even though the true underlying data came from a quadratic model (order = 2), estimated polynomial curves for orders 2, 3 and 4 have relatively low training and test MSE

Polynomial curve of order 1 (linear curves) have high training and test MSE => underfitting

Q2

This question further explores linear regression and ridge regression. The following data pairs are used for training and testing:

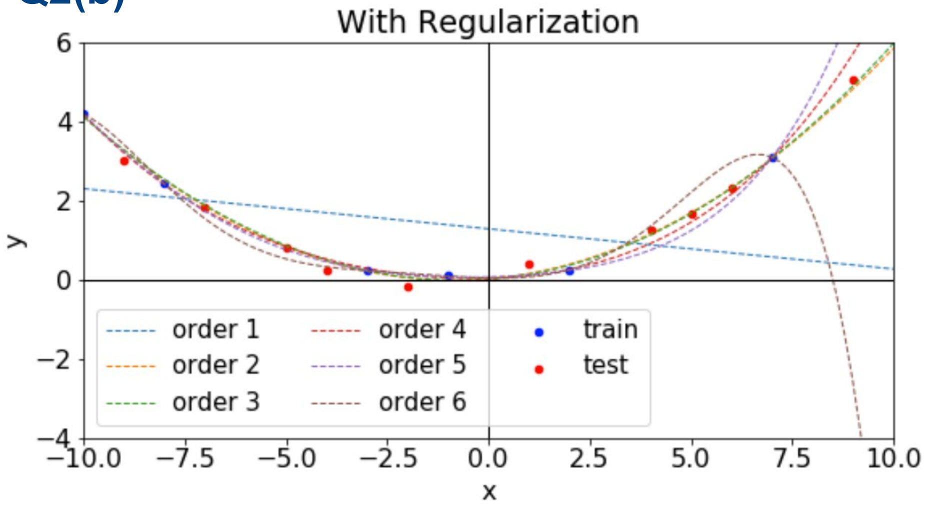
b) Use regularization (ridge regression) $\lambda = 1$ for all orders and repeat the same analyses. Compare the plots of (a) and (b). What do you see?

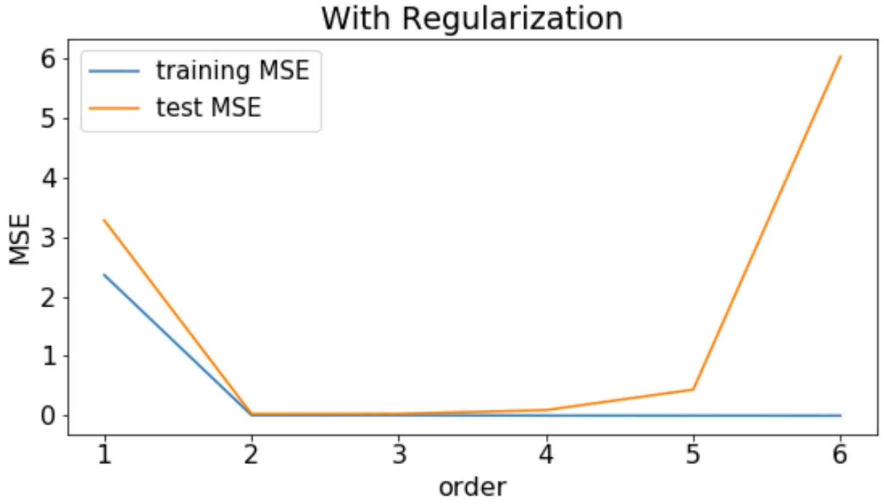
Q2(b)

With regularization, we can simply use the primal solution even for order 6: $\hat{w} = (P^T P + \lambda I)^{-1} P^T y$

```
====== Regularization =======
Training MSE:  [2.3586   8.4565e-03   8.3560e-03   1.8080e-03   7.2650e-04   1.9348e-04]
Test MSE:      [3.2756   0.0302       0.0314       0.0939       0.4369       6.0202]
```

Q2(b)

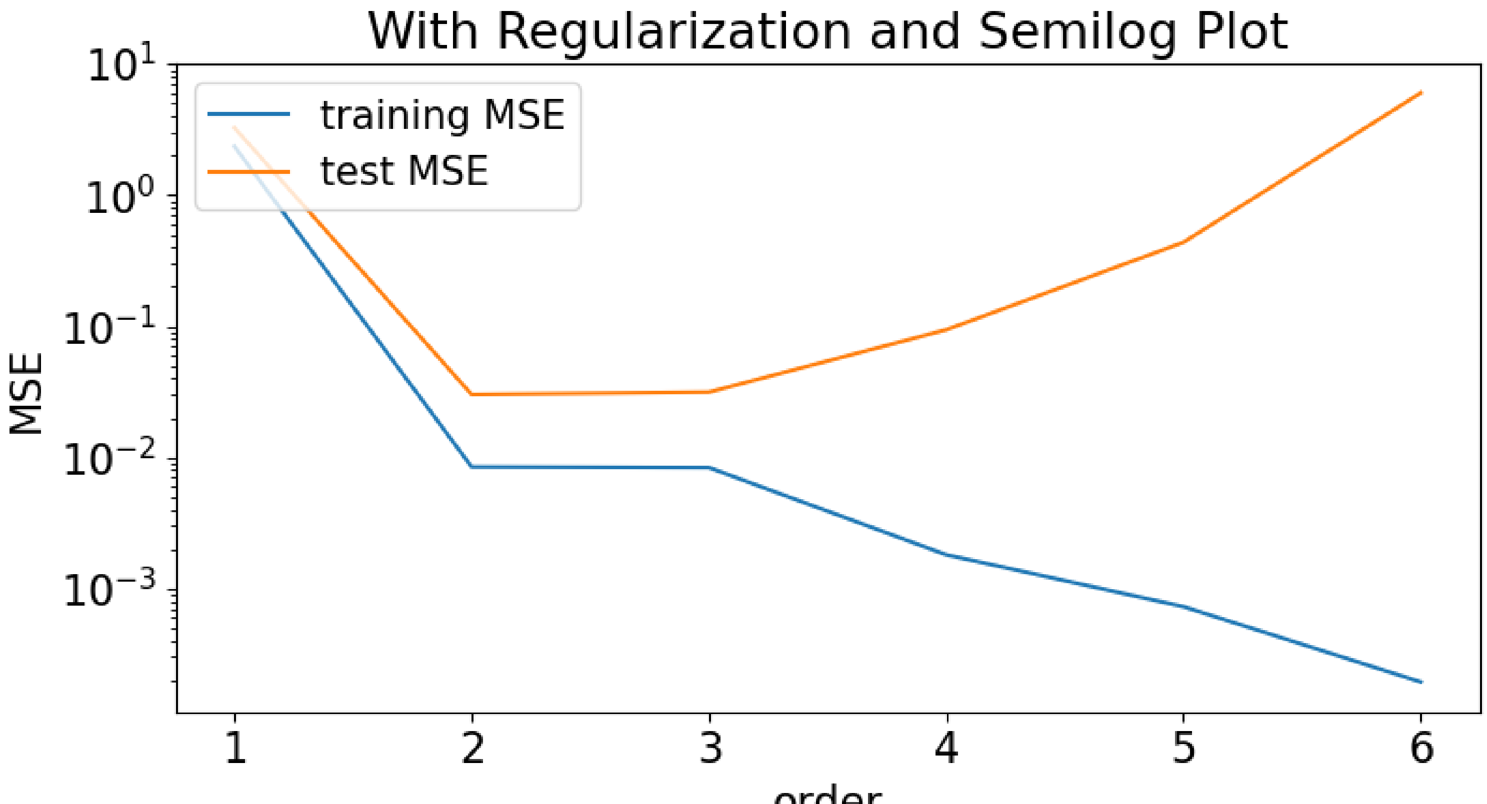




With the regularization, none of the polynomial curves passes through the training samples exactly. In the case of orders 5 and 6, test MSE dropped from 1.0548 (order 5) and 10.7674 (order 6) to 0.4369 (order 5) and 6.0202 (order 6) after regularization was added. Thus, the regularization reduces the overfitting

On the other hand, the regularization did not help orders 1 to 4. Observe that the test MSE actually went up. In this case, the regularization was overly strong, which ended up hurting these orders

Semilog Plot



THANK YOU