Machine Learning - Homework 3

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Pen and Paper Exercises

1st Question

Dataset

In this exercise we aim to learn a regression model for the following dataset:

Observation	x_0	x_1	x_2	output - z
$\vec{x}_1$	1	0.7	-0.3	0.8
$\vec{x}_2$	1	0.4	0.5	0.6
$\vec{x}_3$	1	-0.2	0.8	0.3
$\vec{x}_4$	1	-0.4	0.3	0.3

Table 1: Dataset

$$X = \begin{bmatrix} 1 & 0.7 & -0.3 \\ 1 & 0.4 & 0.5 \\ 1 & -0.2 & 0.8 \\ 1 & -0.4 & 0.3 \end{bmatrix} \qquad Z = \begin{bmatrix} 0.8 \\ 0.6 \\ 0.3 \\ 0.3 \end{bmatrix}$$

$$\vec{x}_1 = \begin{bmatrix} 0.7 \\ -0.3 \end{bmatrix} \qquad \vec{x}_2 = \begin{bmatrix} 0.4 \\ 0.5 \end{bmatrix} \qquad \vec{x}_3 = \begin{bmatrix} -0.2 \\ 0.8 \end{bmatrix} \qquad \vec{x}_4 = \begin{bmatrix} -0.4 \\ 0.3 \end{bmatrix}$$

a)

Transforming the data

We are transforming our original data into a new space, according to the radial basis function:

$$\phi_j(\vec{x}) = \exp\left(-\frac{||\vec{x} - c_j||^2}{2}\right)$$

$$c_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad c_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \qquad c_3 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

After applying the transformation, we will have 3 new inputs for each observation. Therefore, the new dataset will look like:

$$\Phi(X) = X_{trans} = \begin{bmatrix} 1 & \phi_1(\vec{x}_1) & \phi_2(\vec{x}_1) & \phi_3(\vec{x}_1) \\ 1 & \phi_1(\vec{x}_2) & \phi_2(\vec{x}_2) & \phi_3(\vec{x}_2) \\ 1 & \phi_1(\vec{x}_3) & \phi_2(\vec{x}_3) & \phi_3(\vec{x}_3) \\ 1 & \phi_1(\vec{x}_4) & \phi_2(\vec{x}_4) & \phi_3(\vec{x}_4) \end{bmatrix}$$

Observation 1 If we apply our transformation to the first observation $\vec{x}_1$, we get:

$$\phi_1(\vec{x}_1) = \exp\left(-\frac{||\vec{x}_1 - c_1||^2}{2}\right) = \exp\left(-\frac{0.58}{2}\right) = 0.74826$$

$$\phi_2(\vec{x}_1) = \exp\left(-\frac{||\vec{x}_1 - c_2||^2}{2}\right) = \exp\left(-\frac{0.58}{2}\right) = 0.74826$$

$$\phi_3(\vec{x}_1) = \exp\left(-\frac{||\vec{x}_1 - c_3||^2}{2}\right) = \exp\left(-\frac{4.58}{2}\right) = 0.10127$$

Observation 2 If we apply our transformation to the second observation $\vec{x}_2$, we get:

$$\phi_1(\vec{x}_2) = \exp\left(-\frac{||\vec{x}_2 - c_1||^2}{2}\right) = \exp\left(-\frac{0.41}{2}\right) = 0.81465$$

$$\phi_2(\vec{x}_2) = \exp\left(-\frac{||\vec{x}_2 - c_2||^2}{2}\right) = \exp\left(-\frac{2.61}{2}\right) = 0.27117$$

$$\phi_3(\vec{x}_2) = \exp\left(-\frac{||\vec{x}_2 - c_3||^2}{2}\right) = \exp\left(-\frac{2.21}{2}\right) = 0.33121$$

Observation 3 If we apply our transformation to the third observation $\vec{x}_3$, we get:

$$\phi_1(\vec{x}_3) = \exp\left(-\frac{||\vec{x}_3 - c_1||^2}{2}\right) = \exp\left(-\frac{0.68}{2}\right) = 0.71177$$

$$\phi_2(\vec{x}_3) = \exp\left(-\frac{||\vec{x}_3 - c_2||^2}{2}\right) = \exp\left(-\frac{4.68}{2}\right) = 0.09633$$

$$\phi_3(\vec{x}_3) = \exp\left(-\frac{||\vec{x}_3 - c_3||^2}{2}\right) = \exp\left(-\frac{0.68}{2}\right) = 0.71177$$

Observation 4 If we apply our transformation to the fourth observation $\vec{x}_4$, we get:

$$\phi_1(\vec{x}_4) = \exp\left(-\frac{||\vec{x}_4 - c_1||^2}{2}\right) = \exp\left(-\frac{0.25}{2}\right) = 0.88250$$

$$\phi_2(\vec{x}_4) = \exp\left(-\frac{||\vec{x}_4 - c_2||^2}{2}\right) = \exp\left(-\frac{3.65}{2}\right) = 0.16122$$

$$\phi_3(\vec{x}_4) = \exp\left(-\frac{||\vec{x}_4 - c_3||^2}{2}\right) = \exp\left(-\frac{0.85}{2}\right) = 0.65377$$

Transformed Dataset

After applying the transformation, we get the following dataset:

$$\Phi(X) = X_{trans} = \begin{bmatrix} 1 & 0.74826 & 0.74826 & 0.10127 \\ 1 & 0.81465 & 0.27117 & 0.33121 \\ 1 & 0.71177 & 0.09633 & 0.71177 \\ 1 & 0.88250 & 0.16122 & 0.65377 \end{bmatrix}$$

Observation	ϕ_0	ϕ_1	ϕ_2	ϕ_3	output - z
$\vec{x}_1$	1	0.74826	0.74826	0.10127	0.8
$\vec{x}_2$	1	0.81465	0.27117	0.33121	0.6
$\vec{x}_3$	1	0.71177	0.09633	0.71177	0.3
$\vec{x}_4$	1	0.88250	0.16122	0.65377	0.3

Table 2: Transformed Dataset

Ridge Regression

A regression model is characterized by a column matrix of weights W - if we multiply W by a new observation, we get the estimated output for that observation.

$$\hat{z} = w_0 + \sum_{j=1}^{M} w_j x_j = X \cdot W$$

X is the matrix of observations, and W is the matrix of weights:

$$X = \begin{bmatrix} 1 & \vec{x}_1^T \\ 1 & \vec{x}_2^T \\ 1 & \vec{x}_3^T \\ 1 & \vec{x}_4^T \end{bmatrix} \qquad W = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \end{bmatrix}$$

When considering the case where we **transform** our data according to a function ϕ, the regression formula is:

$$\hat{z} = w_0 + \sum_{j=1}^{M} w_j \phi_j(x) = \Phi(X) \cdot W$$

The Ridge Regression (l_2 regularization) is a method that penalizes the weights of the model, in order to avoid overfitting. The formula for W matrix in the Ridge Regression is:

$$W = (\Phi^T \Phi + \lambda I)^{-1} \Phi^T Z$$

Where λ is the regularization parameter ($\lambda = 0.1$), I is the identity matrix and Φ is the matrix of transformed observations.

Computing the weights

Using the formula for W, we get:

$$\Phi = \begin{bmatrix} 1 & 0.74826 & 0.74826 & 0.10127 \\ 1 & 0.81465 & 0.27117 & 0.33121 \\ 1 & 0.71177 & 0.09633 & 0.71177 \\ 1 & 0.88250 & 0.16122 & 0.65377 \end{bmatrix} \quad Z = \begin{bmatrix} 0.8 \\ 0.6 \\ 0.3 \\ 0.3 \end{bmatrix} \quad \Phi^T = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0.74826 & 0.81465 & 0.71177 & 0.88250 \\ 0.74826 & 0.27117 & 0.09633 & 0.16122 \\ 0.10127 & 0.33121 & 0.71177 & 0.65377 \end{bmatrix}$$

$$(\Phi^T \Phi - \lambda I)^{-1} = \begin{bmatrix} 4.54826 & -3.77682 & -1.86117 & -1.86155 \\ -3.77682 & 5.98285 & -0.88543 & -1.26432 \\ -1.86117 & -0.88543 & 4.33276 & 2.72156 \\ -1.86155 & -1.26432 & 2.72156 & 4.53204 \end{bmatrix}$$

$$W = (\Phi^T \Phi + \lambda I)^{-1} \Phi^T Z = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \end{bmatrix} = \begin{bmatrix} 0.33914 \\ 0.19945 \\ 0.40096 \\ -0.29600 \end{bmatrix}$$

Final form of the prediction function

In order to compute $\hat{z}$, we need to multiply the weights by the transformed observation:

$$\hat{z} = \sum_{j=0}^{3} w_j \phi_j(x) = \Phi(X) \cdot W \Leftrightarrow$$

$$\Leftrightarrow \hat{z} = w_0 + w_1 \cdot \phi_1 + w_2 \cdot \phi_2 + w_3 \cdot \phi_3 = 0.33914 + 0.19945 \cdot \phi_1 + 0.40096 \cdot \phi_2 - 0.29600 \cdot \phi_3$$

Using our dataset, the predicted values are:

$$\hat{z} = \begin{bmatrix} 0.75844 \\ 0.51232 \\ 0.30905 \\ 0.38629 \end{bmatrix}$$

b)

The RMSE (Root Mean Squared Error) is a metric that measures the difference between the predicted values and the actual values. It is defined as:

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(z_i - \hat{z}_i)^2}$$

Where z_i is the actual value and $\hat{z}_i$ is the predicted value. In our case, we have the following data:

z_i	$\hat{z}_i$
0.8	0.75844
0.6	0.51232
0.3	0.30905
0.3	0.38629

Table 3: Actual and Predicted Values

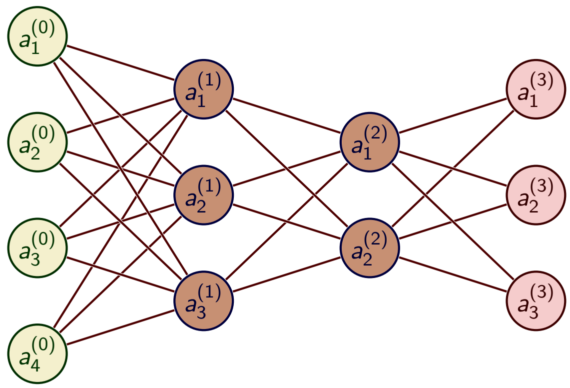
The RMSE is:

$$RMSE = \sqrt{\frac{1}{4}\sum_{i=1}^{4}(z_i - \hat{z}_i)^2} = \sqrt{\frac{1}{4} \cdot 0.01694} = 0.06508$$

2nd Question

Structure of the Network

We are considering a MLP (Multi-Layer Perceptron) with 2 hidden layers. The input and output layers each have 3 neurons. Our structure is the following:



Activation Function

The activation function is the hyperbolic tangent function and it is the same for all layers:

$$f(x) = \tanh(0.5x - 2)$$

$$f'(x) = \frac{1}{\cosh^2(0.5x - 2)}$$

Loss Function

The loss function is the mean square error:

$$E(W) = \frac{1}{2}\sum_{i=1}^{N}(z_i - \hat{z}_i)^2$$