Aprendizagem

LEIC IST-UL

RELATÓRIO - HOMEWORK 3

Grupo 10:

Gabriel Ferreira 107030

Irell Zane 107161

2024/2025 – 1st Semester, P1

Part I: Pen and paper

1. Given the polynomial basis function:

$$\phi(y_1, y_2) = y_1 \times y_2$$

We apply this to our input data:

$$\begin{aligned}
x_1 &: \phi(1,1) = 1 \times 1 = 1 \\
x_2 &: \phi(1,3) = 1 \times 3 = 3 \\
x_3 &: \phi(3,2) = 3 \times 2 = 6 \\
x_4 &: \phi(3,3) = 3 \times 3 = 9 \\
x_5 &: \phi(2,4) = 2 \times 4 = 8
\end{aligned}$$

For OLS, we need $\mathbf{X}$ (input) and $\mathbf{y}$ (output) matrices:

$$\mathbf{X} = \begin{bmatrix} 1 & 1 \\ 1 & 3 \\ 1 & 6 \\ 1 & 9 \\ 1 & 8 \end{bmatrix}$$

$$\mathbf{z} = \begin{bmatrix} 1.25 \\ 7.0 \\ 2.7 \\ 3.2 \\ 5.5 \end{bmatrix}$$

OLS closed form solution calculation

The OLS closed form solution is given by:

$$\boldsymbol{w} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{z}$$

Calculation of the separate components of formula:

$$\mathbf{X}^T\mathbf{X} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 3 & 6 & 9 & 8 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 3 \\ 1 & 6 \\ 1 & 9 \\ 1 & 8 \end{bmatrix} = \begin{bmatrix} 5 & 27 \\ 27 & 191 \end{bmatrix}$$

$$(\mathbf{X}^T\mathbf{X})^{-1} \approx \begin{bmatrix} 0.845 & -0.119 \\ -0.119 & 0.022 \end{bmatrix}$$

$$\mathbf{X}^T\mathbf{z} = \begin{bmatrix} 19.65 \\ 111.25 \end{bmatrix}$$

Finally,

$$\begin{aligned} \boldsymbol{w} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{z} \\ &= \begin{bmatrix} 0.845 & -0.119 \\ -0.119 & 0.022 \end{bmatrix} \times \begin{bmatrix} 19.65 \\ 111.25 \end{bmatrix} \\ &\approx \begin{bmatrix} 3.316 \\ 0.114 \end{bmatrix} \end{aligned}$$

Therefore, the regression model in the transformed space is:

$$y_{num} = 3.316 + 0.114 \times \phi(y_1, y_2)$$

2. **Ridge regression closed form solution calculation**
The ridge regression closed form solution with penalty factor $\lambda = 1$ is given by:

$$\boldsymbol{w} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{z}$$

Calculation of the separate components of formula:

$$\mathbf{X}^T\mathbf{X} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 3 & 6 & 9 & 8 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 3 \\ 1 & 6 \\ 1 & 9 \\ 1 & 8 \end{bmatrix} = \begin{bmatrix} 5 & 27 \\ 27 & 191 \end{bmatrix}$$

$$\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I} = \begin{bmatrix} 5 & 27 \\ 27 & 191 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 6 & 27 \\ 27 & 192 \end{bmatrix}$$

$$(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1} \approx \begin{bmatrix} 0.454 & -0.064 \\ -0.064 & 0.014 \end{bmatrix}$$

$$\mathbf{X}^T\mathbf{z} = \begin{bmatrix} 19.65 \\ 111.25 \end{bmatrix}$$

Finally,

$$\begin{aligned} \boldsymbol{w} &= (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{z} \\ &= \begin{bmatrix} 0.454 & -0.064 \\ -0.064 & 0.014 \end{bmatrix} \times \begin{bmatrix} 19.65 \\ 111.25 \end{bmatrix} \\ &\approx \begin{bmatrix} 1.818 \\ 0.324 \end{bmatrix} \end{aligned}$$

Therefore, the ridge regression model in the transformed space with $\sigma = 1$ is:

$$y_{num} = 1.818 + 0.324 \times \phi(y_1, y_2)$$

The impact of ridge regression on the coefficients can be observed by comparing the Ordinary Least Squares (OLS) solution with the ridge regression solution (using $\lambda = 1$):

$$\text{OLS coefficients:} \quad \boldsymbol{w}_{\text{OLS}} \approx \begin{bmatrix} 3.316 \\ 0.114 \end{bmatrix}$$

$$\text{Ridge coefficients:} \quad \boldsymbol{w}_{\text{Ridge}} \approx \begin{bmatrix} 1.818 \\ 0.324 \end{bmatrix}$$

The effects of ridge regression are as follows: The larger coefficient (intercept) has been substantially reduced from 3.316 to 1.818. The smaller coefficient increased from. This aligns with the primary goal of ridge regression to shrink large coefficients, which are more heavily penalized due to the quadratic regularization term.

Ultimately the Ridge regression has reduced the sum of squared coefficients:

$$\begin{aligned} \text{OLS:} &\quad 3.316^2 + 0.114^2 \approx 11.00 \\ \text{Ridge:} &\quad 1.818^2 + 0.324^2 \approx 3.41 \end{aligned}$$

This significant reduction in the sum of squared coefficients indicates a less complex model, which is likely to generalize better to unseen data.

3. **OLS and Ridge prediction calculations**

For $x_1 = (1, 1)$:

$$\begin{aligned} \phi(1,1) &= 1 \times 1 = 1 \\ y_{OLS} &= 3.316 + 0.114 \times 1 = 3.430 \\ y_{Ridge} &= 1.818 + 0.324 \times 1 = 2.142 \end{aligned}$$

For $x_2 = (1, 3)$:

$$\begin{aligned} \phi(1,3) &= 1 \times 3 = 3 \\ y_{OLS} &= 3.316 + 0.114 \times 3 = 3.658 \\ y_{Ridge} &= 1.818 + 0.324 \times 3 = 2.790 \end{aligned}$$

For $x_3 = (3, 2)$:

$$\begin{aligned}\phi(3,2) &= 3 \times 2 = 6\\ y_{OLS} &= 3.316 + 0.114 \times 6 = 4.000\\ y_{Ridge} &= 1.818 + 0.324 \times 6 = 3.762\end{aligned}$$

For $x_4 = (3, 3)$:

$$\begin{aligned}\phi(3,3) &= 3 \times 3 = 9\\ y_{OLS} &= 3.316 + 0.114 \times 9 = 4.342\\ y_{Ridge} &= 1.818 + 0.324 \times 9 = 4.734\end{aligned}$$

For $x_5 = (2, 4)$:

$$\begin{aligned}\phi(2,4) &= 2 \times 4 = 8\\ y_{OLS} &= 3.316 + 0.114 \times 8 = 4.228\\ y_{Ridge} &= 1.818 + 0.324 \times 8 = 4.410\end{aligned}$$

For $x_6 = (2, 2, 0.7)$:

$$\begin{aligned}\phi(2,2) &= 2 \times 2 = 4\\ y_{OLS} &= 3.316 + 0.114 \times 4 = 3.772\\ y_{Ridge} &= 1.818 + 0.324 \times 4 = 3.114\end{aligned}$$

For $x_7 = (1, 2, 1.1)$:

$$\begin{aligned}\phi(1,2) &= 1 \times 2 = 2\\ y_{OLS} &= 3.316 + 0.114 \times 2 = 3.544\\ y_{Ridge} &= 1.818 + 0.324 \times 2 = 2.466\end{aligned}$$

For $x_8 = (5, 1, 2.2)$:

$$\begin{aligned}\phi(5,1) &= 5 \times 1 = 5\\ y_{OLS} &= 3.316 + 0.114 \times 5 = 3.886\\ y_{Ridge} &= 1.818 + 0.324 \times 5 = 3.438\end{aligned}$$

Train RMSE calculation

$$
\begin{aligned}
RMSE_{OLS} &= \sqrt{\frac{1}{5}\sum_{i=1}^{5}(y_i - \hat{y}_i)^2} \\
&= \sqrt{\frac{1}{5}[(1.25 - 3.430)^2 + (7 - 3.658)^2 + (2.7 - 4.000)^2 + (3.2 - 4.342)^2 + (5.5 - 4.228)^2]} \\
&= \sqrt{\frac{1}{5}[(-2.180)^2 + (3.342)^2 + (-1.300)^2 + (-1.142)^2 + (1.272)^2]} \\
&= \sqrt{\frac{1}{5}[4.7524 + 11.1697 + 1.6900 + 1.3042 + 1.6188]} \\
&= \sqrt{\frac{1}{5} \times 20.5351} \\
&\approx 2.027
\end{aligned}
$$

$$
\begin{aligned}
RMSE_{Ridge} &= \sqrt{\frac{1}{5}\sum_{i=1}^{5}(y_i - \hat{y}_i)^2} \\
&= \sqrt{\frac{1}{5}[(1.25 - 2.142)^2 + (7 - 2.790)^2 + (2.7 - 3.762)^2 + (3.2 - 4.734)^2 + (5.5 - 4.410)^2]} \\
&= \sqrt{\frac{1}{5}[(-0.892)^2 + (4.210)^2 + (-1.062)^2 + (-1.534)^2 + (1.090)^2]} \\
&= \sqrt{\frac{1}{5}[0.7953 + 17.7321 + 1.1278 + 2.3524 + 1.1881]} \\
&= \sqrt{\frac{1}{5} \times 23.1957} \\
&\approx 2.154
\end{aligned}
$$

Test RMSE calculation

$$
\begin{aligned}
RMSE_{OLS} &= \sqrt{\frac{1}{3}\sum_{i=6}^{8}(y_i - \hat{y}_i)^2} \\
&= \sqrt{\frac{1}{3}[(0.7 - 3.772)^2 + (1.1 - 3.544)^2 + (2.2 - 3.886)^2]} \\
&\approx 2.467
\end{aligned}
$$

$$
\begin{aligned}
RMSE_{Ridge} &= \sqrt{\frac{1}{3}\sum_{i=6}^{8}(y_i - \hat{y}_i)^2} \\
&= \sqrt{\frac{1}{3}[(0.7 - 3.114)^2 + (1.1 - 2.466)^2 + (2.2 - 3.438)^2]} \\
&\approx 1.748
\end{aligned}
$$

The results show that the Ridge regression model has a lower test RMSE and a higher train RMSE compared to the original OLS model for the given train data. This shows that the original OLS model overfits more than the Ridge regression model. This aligns with our expectations as the objective of the regularization in ridge regression was so that the model overfits the training data less and generalize better for unseen data.

4. **MLP Propagation:**

$$
x^{[1]} = z^{[1]} = W^{[1]}x^{[0]} + b^{[1]} = \begin{pmatrix} 0.1 & 0.1 \\ 0.1 & 0.2 \\ 0.2 & 0.1 \end{pmatrix} \begin{pmatrix} 1 & 1 \end{pmatrix} + \begin{pmatrix} 0.1 \\ 0 \\ 0.1 \end{pmatrix} = \begin{pmatrix} 0.3 \\ 0.3 \\ 0.4 \end{pmatrix}
$$

$$
z^{[2]} = W^{[2]}x^{[1]} + b^{[2]} = \begin{pmatrix} 1 & 2 & 2 \\ 1 & 2 & 1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 0.3 \\ 0.3 \\ 0.4 \end{pmatrix} + \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 2.7 \\ 2.3 \\ 2 \end{pmatrix}
$$

$$
x^{[2]} = softmax(z^{[2]}) = \begin{pmatrix} 0.46 \\ 0.31 \\ 0.23 \end{pmatrix}
$$

Backpropagation:

$$
\delta^{[2]} = \frac{\partial E}{\partial x^{[2]}} \circ \frac{\partial x^{[2]}}{\partial z^{[2]}} = x^{[2]} - t = \begin{pmatrix} 0.46 - 0 \\ 0.31 - 1 \\ 0.23 - 0 \end{pmatrix} = \begin{pmatrix} 0.46 \\ -0.69 \\ 0.23 \end{pmatrix}
$$

Layer 2 weights:

$$
\frac{\partial E}{\partial W^{[2]}} = \delta^{[2]}(x^{[1]})^T = \begin{pmatrix} 0.46 \\ -0.69 \\ 0.23 \end{pmatrix} \begin{pmatrix} 0.3 & 0.3 & 0.4 \end{pmatrix} = \begin{pmatrix} 0,14 & 0,14 & 0,18 \\ -0,21 & -0,21 & -0,28 \\ 0,07 & 0,07 & 0,09 \end{pmatrix}
$$

$$
W^{[2]}_{new} = W^{[2]}_{old} - \eta \frac{\partial E}{\partial W^{[2]}} = \begin{pmatrix} 1 & 2 & 2 \\ 1 & 2 & 1 \\ 1 & 1 & 1 \end{pmatrix} - 0.1 \begin{pmatrix} 0.81 & 0.81 & 1.08 \\ 0.39 & 0.39 & 0.52 \\ 0.6 & 0.6 & 0.8 \end{pmatrix} = \begin{pmatrix} 0.99 & 1.99 & 1.98 \\ 1.02 & 2.02 & 1.03 \\ 0.99 & 0.99 & 0.99 \end{pmatrix}
$$

Layer 2 biases:

$$\frac{\partial E}{\partial b^{[2]}} = \delta^{[2]} \frac{\partial z^{[2]}}{\partial b^{[2]}}^T = \delta^{[2]} = \begin{pmatrix} 0.46 \\ -0.69 \\ 0.23 \end{pmatrix}$$

$$b^{[2]}_{new} = b^{[2]}_{old} - \eta \frac{\partial E}{\partial b^{[2]}} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} - 0.1 \begin{pmatrix} 0.46 \\ -0.69 \\ 0.23 \end{pmatrix} = \begin{pmatrix} 0.95 \\ 1.07 \\ 0.98 \end{pmatrix}$$

Layer 1 weights:

$$\delta^{[1]} = \left(\frac{\partial z^{[2]}}{\partial x^{[1]}}\right)^T \cdot \delta^{[2]} \circ \frac{\partial x^{[1]}}{\partial z^{[1]}} = (W^{[2]})^T \delta^{[2]} \times 1 = \begin{pmatrix} 0.00 \\ -0.23 \\ 0.46 \end{pmatrix}$$

$$\frac{\partial E}{\partial W^{[1]}} = \delta^{[1]} (x^{[0]})^T = \begin{pmatrix} 0.00 \\ -0.23 \\ 0.46 \end{pmatrix} \begin{pmatrix} 1 & 1 \end{pmatrix} = \begin{pmatrix} 0.00 & 0.00 \\ -0.23 & -0.23 \\ 0.46 & 0.46 \end{pmatrix}$$

$$W^{[1]}_{new} = W^{[1]}_{old} - \eta \frac{\partial E}{\partial W^{[1]}} = \begin{pmatrix} 0.1 & 0.1 \\ 0.1 & 0.2 \\ 0.2 & 0.1 \end{pmatrix} - 0.1 \begin{pmatrix} 0.00 & 0.00 \\ -0.23 & -0.23 \\ 0.46 & 0.46 \end{pmatrix} = \begin{pmatrix} 0.10 & 0.10 \\ 0.12 & 0.22 \\ 0.15 & 0.05 \end{pmatrix}$$

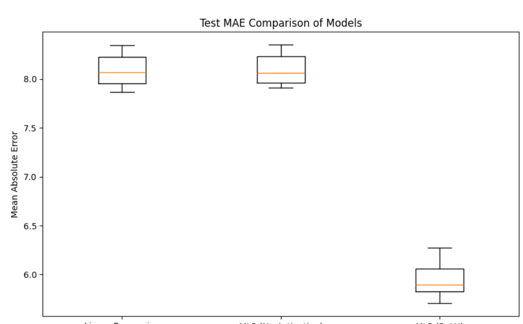
Layer 1 biases:

$$\frac{\partial E}{\partial b^{[1]}} = \delta^{[1]} \frac{\partial z^{[1]}}{\partial b^{[1]}}^T = \delta^{[1]} = \begin{pmatrix} 0.00 \\ -0.23 \\ 0.46 \end{pmatrix}$$

$$b^{[1]}_{new} = b^{[1]}_{old} - \eta \frac{\partial E}{\partial b^{[1]}} = \begin{pmatrix} 0.1 \\ 0 \\ 0.1 \end{pmatrix} - 0.1 \begin{pmatrix} 0.00 \\ -0.23 \\ 0.46 \end{pmatrix} = \begin{pmatrix} 0.10 \\ 0.02 \\ 0.05 \end{pmatrix}$$

Part II: Programming

5. Model's boxplots.



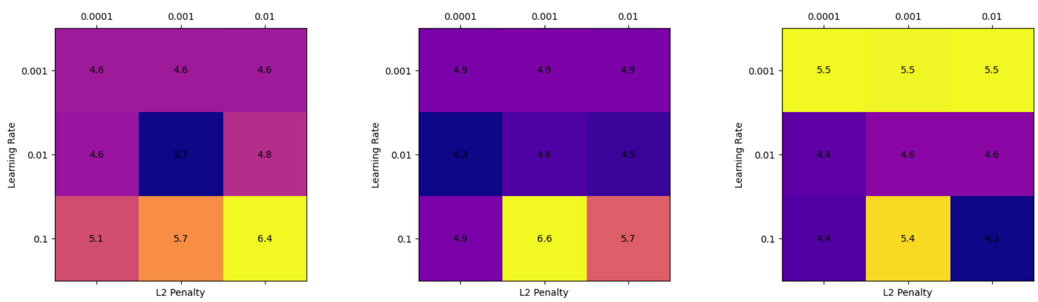
6. Comparison.

   As we can see, Linear Regression and MLP with no activation perform pratically the same, even with 2 hidden layers of 10 neurons.

   The main problem with using no activation in the MLP, this is, using the linear unit, is that the model will be unable to approximate non-linear functions well, this is because an MLP without activation is in practice equivalent to linear regression.

   This is corroborated by the box plot, as no activation MLP performs similarly to Linear Regression, but MLP with a Rectified LU activation performs much better with a smaller MAE.

7. Grid Search.



(a) Batch size: 32 (b) Batch size: 64 (c) Batch size: 128

   According to our grid search, the best combination of hyperparameters seems to be a batch size of 32, a learning rate of 0.01 and a L2 Penalty of 0.001. With the 80-20 train-test split it performed with a Mean Absolute Error of 3.7 which is below the alternatives.

   With a very low learning rate of 0.001 the model doesn't seem to perform very well, and seems to not be affected by the L2 Penalty, this might be because it converges very little, since it stops at 200 iterations.

   A learning rate of 0.01 seems to perform usually the best, while a learning rate of 0.1 is, as expected, more chaotic than the rest. The batch size doesn't seem to have a big impact but smaller learning rates perform better with smaller batch sizes and larger batch sizes with greater learning rates.