Aprendizagem 2022/23

Homework III

Deadline 28/10/2022 23:59 via Fenix as PDF

1)

Design Matrix :

$$X = \begin{array}{c} \begin{array}{cccc} \text{Bias} & & & \\ \downarrow & & & \end{array} \\ \begin{pmatrix} 1 & x_1^1 & x_1^2 & x_1^3 \\ 1 & x_2^1 & x_2^2 & x_2^3 \\ 1 & x_3^1 & x_3^2 & x_3^3 \\ 1 & x_4^1 & x_4^2 & x_4^3 \\ 1 & x_5^1 & x_5^2 & x_5^3 \end{pmatrix} \end{array} = \begin{pmatrix} 1 & 0.8 & 0.64 & 0.512 \\ 1 & 1 & 1 & 1 \\ 1 & 1.2 & 1.44 & 1.728 \\ 1 & 1.4 & 1.96 & 2.744 \\ 1 & 1.6 & 2.56 & 4.096 \end{pmatrix}$$

$$X^T = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 0.8 & 1 & 1.2 & 1.4 & 1.6 \\ 0.64 & 1 & 1.44 & 1.96 & 2.56 \\ 0.512 & 1 & 1.728 & 2.744 & 4.096 \end{pmatrix}$$

$4 \times 5 \quad 5 \times 4$

$$X^T X = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 0.8 & 1 & 1.2 & 1.4 & 1.6 \\ 0.64 & 1 & 1.44 & 1.96 & 2.56 \\ 0.512 & 1 & 1.728 & 2.744 & 4.096 \end{pmatrix} \begin{pmatrix} 1 & 0.8 & 0.64 & 0.512 \\ 1 & 1 & 1 & 1 \\ 1 & 1.2 & 1.44 & 1.728 \\ 1 & 1.4 & 1.96 & 2.744 \\ 1 & 1.6 & 2.56 & 4.096 \end{pmatrix}$$

$$= \begin{pmatrix} 5 & 6 & 7.6 & 10.08 \\ 6 & 7.6 & 10.08 & 13.8784 \\ 7.6 & 10.08 & 13.8784 & 19.68 \\ 10.08 & 13.8784 & 19.68 & 28.55488 \end{pmatrix}$$

$$(X^TX+\lambda I)^{-1} = \left[\begin{pmatrix} 5 & 6 & 7.6 & 10.08 \\ 6 & 7.6 & 10.08 & 13.8784 \\ 7.6 & 10.08 & 13.8784 & 19.68 \\ 10.08 & 13.8784 & 19.68 & 28.55488 \end{pmatrix} + \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}\right]^{-1}$$

$$= \begin{pmatrix} 7 & 6 & 7.6 & 10.08 \\ 6 & 9.6 & 10.08 & 13.8784 \\ 7.6 & 10.08 & 15.8784 & 19.68 \\ 10.08 & 13.8784 & 19.68 & 30.55488 \end{pmatrix}^{-1}$$

$$= \begin{pmatrix} 0.3417 & -0.1214 & -0.0749 & -0.0093 \\ -0.1214 & 0.3892 & -0.0967 & -0.0745 \\ -0.0749 & -0.0967 & 0.3726 & -0.1714 \\ -0.0093 & -0.0745 & -0.1714 & 0.18 \end{pmatrix}$$

$$(X^TX+\lambda I)^{-1}X^T = \begin{pmatrix} 0.3417 & -0.1214 & -0.0749 & -0.0093 \\ -0.1214 & 0.3892 & -0.0967 & -0.0745 \\ -0.0749 & -0.0967 & 0.3726 & -0.1714 \\ -0.0093 & -0.0745 & -0.1714 & 0.18 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 0.8 & 1 & 1.2 & 1.4 & 1.6 \\ 0.64 & 1 & 1.44 & 1.96 & 2.56 \\ 0.512 & 1 & 1.728 & 2.744 & 4.096 \end{pmatrix}$$

$$= \begin{pmatrix} 0.1918 & 0.136 & 0.072 & -0.0007 & -0.082 \\ 0.9 & 0.0966 & 0.0777 & 0.0296 & -0.051 \\ -0.001 & 0.0296 & 0.0495 & 0.05 & 0.0223 \\ -0.086 & -0.075 & -0.034 & 0.0444 & 0.1701 \end{pmatrix}$$

$$w = (X^TX+\lambda I)^{-1}X^TZ = \begin{pmatrix} 0.1918 & 0.136 & 0.072 & -0.0007 & -0.082 \\ 0.9 & 0.0966 & 0.0777 & 0.0296 & -0.051 \\ -0.001 & 0.0296 & 0.0495 & 0.05 & 0.0223 \\ -0.086 & -0.075 & -0.034 & 0.0444 & 0.1701 \end{pmatrix} \begin{pmatrix} 24 \\ 20 \\ 10 \\ 13 \\ 12 \end{pmatrix}$$

$$= \begin{pmatrix} 7.0451 \\ 4.6409 \\ 1.9673 \\ -1.301 \end{pmatrix}$$

Therefore, the weights of the Ridge Regression are $w = \begin{pmatrix} 7.0451 \\ 4.6409 \\ 1.9673 \\ -1.301 \end{pmatrix}$ //

2) $\hat{z}(x,w) = w_0 + w_1 x + w_2 x^2 + w_3 x^3$

$= 7.0451 + 4.6409\,x + 1.9673\,x^2 - 1.301\,x^3$

$\hat{z}_0 = \hat{z}(x_0, w) = 7.0451 + 4.6409 \times 0.8 + 1.9673 \times 0.8^2 - 1.301 \times 0.8^3$

$= 11.35078$

$\hat{z}_1 = \hat{z}(x_1, w) = 7.0451 + 4.6409 \times 1 + 1.9673 \times 1^2 - 1.301 \times 1^3$

$= 12.3523$

$\hat{z}_2 = \hat{z}(x_2, w) = 7.0451 + 4.6409 \times 1.2 + 1.9673 \times 1.2^2 - 1.301 \times 1.2^3$

$= 13.199$

$\hat{z}_3 = \hat{z}(x_3, w) = 7.0451 + 4.6409 \times 1.4 + 1.9673 \times 1.4^2 - 1.301 \times 1.4^3$

$= 13.8283$

$\hat{z}_4 = \hat{z}(x_4, w) = 7.0451 + 4.6409 \times 1.6 + 1.9673 \times 1.6^2 - 1.301 \times 1.6^3$

$= 14.178$

$$\text{RMSE} = \sqrt{\sum_{i=0}^{4} \frac{(\hat{z}_i - z_i)^2}{5}}$$

$$= \sqrt{\frac{1}{5}\left((\hat{z}_0 - z_0)^2 + (\hat{z}_1 - z_1)^2 + (\hat{z}_2 - z_2)^2 + (\hat{z}_3 - z_3)^2 + (\hat{z}_4 - z_4)^2\right)}$$

$= 6.8433$

The RMSE of the learnt Ridge Regression model is 6.8433 //

3) **1° • Forward Propagation**

$$\rightarrow W^{[1]} = \begin{bmatrix}1\\1\end{bmatrix} \quad \rightarrow b^{[1]} = \begin{bmatrix}1\\1\end{bmatrix}$$

$$\rightarrow w^{[2]} = \begin{bmatrix}1 & 1\end{bmatrix} \quad \rightarrow b^{[2]} = 1$$

$$\rightarrow z^{[i]} = w^{[i]} x^{[i-1]} + b^{[1]}$$

$$\rightarrow x^{[i]} = f(z^{[i]}) = e^{0\,1 z^{[i]}}$$

$x_0^{[0]} = 0.8$

$$z_0^{[1]} = w_0^{[1]} x_0^{[0]} + b_0^{[1]}$$

$$= \begin{bmatrix}1\\1\end{bmatrix} 0.8 + \begin{bmatrix}1\\1\end{bmatrix}$$

$$= \begin{bmatrix}1.8\\1.8\end{bmatrix}$$

$$x_0^{[1]} = f(z_0^{[1]})$$

$$= \begin{bmatrix}1.197\\1.197\end{bmatrix}$$

$$z_0^{[2]} = w_0^{[2]} x_0^{[1]} + b_0^{[2]}$$

$$= \begin{bmatrix}1 & 1\end{bmatrix}\begin{bmatrix}1.197\\1.197\end{bmatrix} + 1$$

$$= 3.394$$

$$x_0^{[2]} = f(z_0^{[2]})$$

$$= 1.4041$$

$x_1^{[0]} = 1$

$$z^{[1]} = w_1^{[1]} x_1^{[0]} + b_1^{[1]}$$

$$= \begin{bmatrix}1\\1\end{bmatrix} 1 + \begin{bmatrix}1\\1\end{bmatrix}$$

$$= \begin{bmatrix}2\\2\end{bmatrix}$$

$$x_1^{[1]} = f(z_1^{[1]})$$

$$= \begin{bmatrix}1.221\\1.221\end{bmatrix}$$

$$z_1^{[2]} = w_1^{[2]} x_1^{[1]} + b_1^{[2]}$$

$$= \begin{bmatrix}1 & 1\end{bmatrix}\begin{bmatrix}1.221\\1.221\end{bmatrix} + 1$$

$$= 3.442$$

$$x_1^{[2]} = f(z_1^{[2]})$$

$$= 1.411$$

$x_2^{[0]} = 1.2$

$$z_2^{[1]} = w_2^{[1]} x_2^{[0]} + b_2^{[1]}$$

$$= \begin{bmatrix}1\\1\end{bmatrix} 1.2 + \begin{bmatrix}1\\1\end{bmatrix}$$

$$= \begin{bmatrix}2.2\\2.2\end{bmatrix}$$

$$x_2^{[1]} = f(z_2^{[1]})$$

$$= \begin{bmatrix}1.246\\1.246\end{bmatrix}$$

$$z_2^{[2]} = w_2^{[2]} x_2^{[1]} + b_2^{[2]}$$

$$= \begin{bmatrix}1 & 1\end{bmatrix}\begin{bmatrix}1.246\\1.246\end{bmatrix} + 1$$

$$= 3.492$$

$$x_2^{[2]} = f(z_2^{[2]})$$

$$= 1.418$$

2° - Backward Propagation

→ $X_0^{[2]} = 1.4041$ → $X_1^{[2]} = 1.411$ → $X_2^{[2]} = 1.418$

→ $T_0 = 24$ → $t_1 = 20$ → $t_2 = 10$

→ $E_j(w^{[i]}) = \frac{1}{2}\left(x_j^{[i]} - t_j\right)^2$

→ $\delta_j^{[i]} = \frac{\partial E}{\partial x^{[i]}} \circ \frac{\partial x^{[i]}}{\partial z^{[i]}}$

$= \left(x_j^{[i]} - t_j\right) \circ 0.1e^{0.1 z_j^{[i]}}$

→ $\delta_j^{[i]} = W^{[i+1]^T} \cdot \delta_j^{[i+1]} \circ 0.1e^{0.1 z_j^{[i]}}$

→ $\delta^{[i]} = \sum_{j=0}^{2} \delta_j^{[i]}$

→ $f'(u) = 0.1e^{0.1u}$

→ $x^{[i]} = f(z^{[i]})$

$\Rightarrow \frac{\partial x^{[i]}}{\partial z^{[i]}} = f'(z^{[i]}) \cdot z^{[i]'}$

$= 0.1e^{0.1 z^{[i]}}$

→ $\frac{\partial E}{\partial w^{[i]}} = \sum_{j=0}^{2} \delta_j^{[i]} \cdot \left(\frac{\partial z_j^{[i]}}{\partial w^{[i]}}\right)^T$

$= \sum_{j=0}^{2} \delta_j^{[i]} \cdot \left(X_j^{[i-1]}\right)^T$

→ $w^{[k]} = w^{[k]} - n \frac{\partial E}{\partial w^{[i]}}$

→ $b^{[k]} = b^{[k]} - n\,\delta^{[k]}$

Calculations

Level 2

$\delta_0^{[2]} = (1.4041 - 24) \times 0.1e^{0.1 \times 3.394}$

$= -3.1727$

$\delta_1^{[2]} = (1.411 - 20) \times 0.1e^{0.1 \times 3.442}$

$= -2.623$

$\delta_2^{[2]} = (1.418 - 10) \times 0.1e^{0.1 \times 3.492}$

$= -1.217$

$$w^{[2]} = w^{[2]} - \eta \boxed{\frac{\partial E}{\partial w^{[2]}}}$$

$$= \sum \delta_i^{[0]} \cdot x_i^{[1]^T}$$

$$= -3.1727 \begin{bmatrix} 1.197 \\ 1.197 \end{bmatrix}^T - 2.623 \begin{bmatrix} 1.221 \\ 1.221 \end{bmatrix}^T - 1.217 \begin{bmatrix} 1.246 \\ 1.246 \end{bmatrix}^T$$

$$= \begin{bmatrix} -8.517 \\ -8.517 \end{bmatrix}^T$$

$$= \begin{bmatrix} 1 & 1 \end{bmatrix} - 0.1 \begin{bmatrix} -8.517 & -8.517 \end{bmatrix}$$

$$= \begin{bmatrix} 1.8517 & 1.8517 \end{bmatrix}$$

$$b^{[2]} = b^{[2]} - \eta \, \delta^{[2]}$$

$$= 1 - 0.1 \left(-3.1727 - 2.623 - 1.217 \right)$$

$$= 1.7013$$

Level 1

$$\delta_0^{[1]} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \times -3.1727 \circ \begin{bmatrix} 0.1e^{0.1 \times 1.8} \\ 0.1e^{0.1 \times 1.8} \end{bmatrix}$$

$$= \begin{bmatrix} -0.38 \\ -0.38 \end{bmatrix}$$

$$\delta_1^{[1]} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \times -2.623 \circ \begin{bmatrix} 0.1e^{0.1 \times 2} \\ 0.1e^{0.1 \times 2} \end{bmatrix}$$

$$= \begin{bmatrix} -0.32 \\ -0.32 \end{bmatrix}$$

$$\delta_2^{[1]} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \times -1.217 \circ \begin{bmatrix} 0.1e^{0.1 \times 2.2} \\ 0.1e^{0.1 \times 2.2} \end{bmatrix}$$

$$= \begin{bmatrix} -0.15 \\ -0.15 \end{bmatrix}$$

$$w^{[1]} = w^{[1]} - \eta \boxed{\frac{\partial E}{\partial w^{[1]}}}$$

$$\shortparallel$$

$$\sum \delta^{[1]} \cdot X^{[0]^T}$$

$$= \begin{bmatrix}-0.38\\-0.38\end{bmatrix} \times 0.8 + \begin{bmatrix}-0.32\\-0.32\end{bmatrix} \times 1 + \begin{bmatrix}-0,15\\-0,15\end{bmatrix} \times 1,2$$

$$= \begin{bmatrix}-0.804\\-0.804\end{bmatrix}$$

$$= \begin{bmatrix}1\\1\end{bmatrix} - 0.1 \begin{bmatrix}-0,804\\-0,804\end{bmatrix}$$

$$= \begin{bmatrix}1.0804\\1.0804\end{bmatrix}$$

$$b^{[1]} = b^{[1]} - \eta\, \delta^{[1]}$$

$$= \begin{bmatrix}1\\1\end{bmatrix} - 0.1 \left(\begin{bmatrix}-0.38\\-0.38\end{bmatrix} + \begin{bmatrix}-0.32\\-0.32\end{bmatrix} + \begin{bmatrix}-0.15\\-0.15\end{bmatrix} \right)$$

$$= \begin{bmatrix}1.0805\\1.0805\end{bmatrix}$$

Therefore, the updated weights and bias are:

$$w^{[2]} = \begin{bmatrix}1.8517 & 1.8517\end{bmatrix} \qquad b^{[2]} = 1,7013$$

$$w^{[1]} = \begin{bmatrix}1.0804\\1.0804\end{bmatrix} \qquad b^{[1]} = \begin{bmatrix}1.0805\\1.0805\end{bmatrix}$$

II. Programming and critical analysis

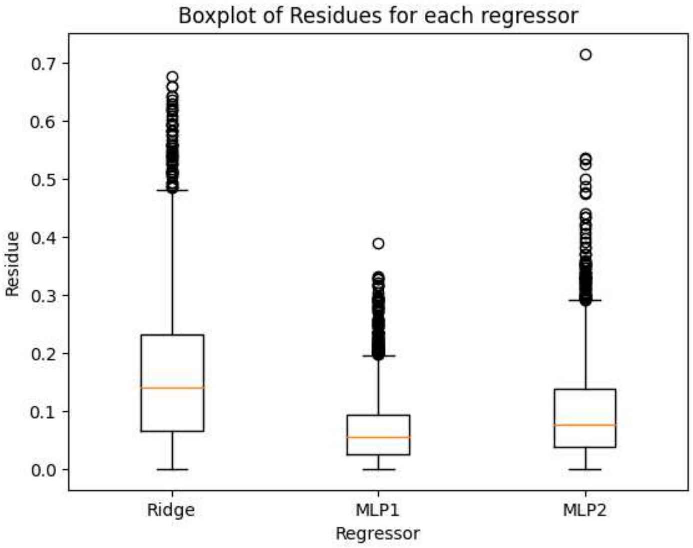
The code for the questions is in the Appendix of this document.

4) Ridge Regression MAE: 0.162829976437694

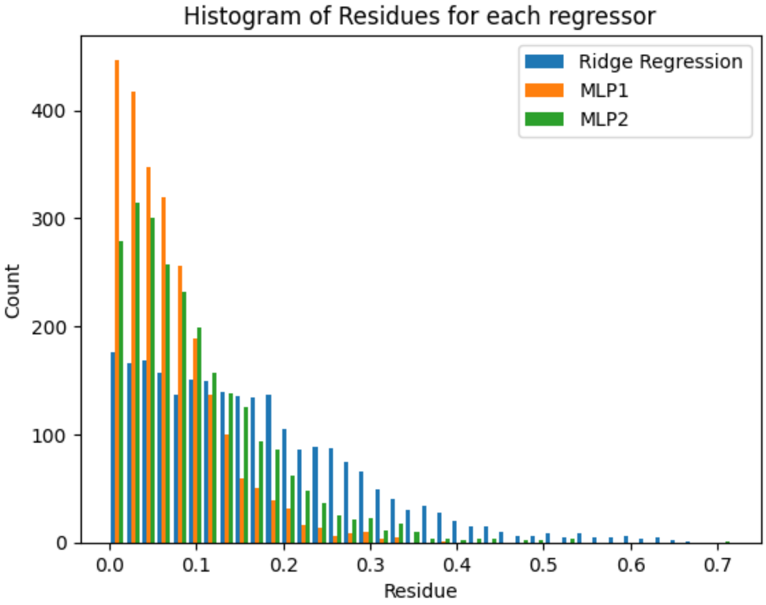
   MAE for MLP1: 0.0680414073796843

   MAE for MLP2: 0.0978071820387748

5) Resulting Boxplot:



Resulting Histogram:



6) MLP1 iterations: 452

MLP2 iterations: 77

7) In a batch gradient descent algorithm, the number of iterations matches the number of epochs run. In this case, the number of iterations required for MLP1 and MLP2 to converge is very different (452 vs 77). This might be related to the fact that MLP1 uses early stopping and MLP2 does not.

Early stopping is a method that stops the training when the validation score is not improving by at least e^{-4} {1} for 10 {2} consecutive epochs and it is done to avoid overfitting.

The validation set may contain samples from both training and test sets since the parameter **`shuffle`** is set to True by default. Therefore, the training process may converge after a different amount of epochs depending on the samples in the validation set.

MLP2 doesn't use early stopping, so it will continue to train until it reaches the maximum number of iterations (500) and, therefore, it is more likely to overfit the data. However, MLP2 stopped at 77 iterations, which is much less than 500.

The difference in the number of iterations required for MLP2 to converge is much lower compared to MLP1, probably, because each model uses a different training set and due to the fact that MLP1 uses early stopping and MLP2 does not.

Since, MLP2 has a higher MAE and is more overfitted than MLP1, we can conclude that MLP1 has a better performance than MLP2.

{1} - default **`tol`** (tolerance) in MLPRegressor function

{2} - default maximum number of epochs to not meet **`tol`** improvement in MLPRegressor function (n_iter_no_change)

III. APPENDIX

Code used in question 4) of **II. Programming and critical analysis**:

Loads the data:

```
import pandas as pd
import numpy as np
from sklearn.linear_model import LinearRegression, Ridge
from sklearn.neural_network import MLPRegressor
from sklearn.metrics import mean_absolute_error
from scipy.io.arff import loadarff
from sklearn import model_selection
from sklearn import metrics

#load data
data = loadarff('kin8nm.arff')
df = pd.DataFrame(data[0])
df.head()
```

Calculates the mean absolute error of the Ridge Regression:

```
#split data
X = df.drop('y', axis=1)
y = df['y']
X_train, X_test, y_train, y_test = model_selection.train_test_split(X.values,
      y.values, train_size=0.7, random_state=0)

#train models and get MAE for Ridge
rr = Ridge(alpha=0.1)
rr.fit(X_train, y_train)
pint('Ridge Regression MAE: ', mean_absolute_error(y_test, rr.predict(X_test)))
```

Calculates the mean absolute errors of the Multi-Layer Perceptrons:

```
#train models and get MAE for MLPs
mlp1 = MLPRegressor(hidden_layer_sizes=(10, 10), activation='tanh',
      max_iter=500, random_state=0, early_stopping=True)
mlp2 = MLPRegressor(hidden_layer_sizes=(10, 10), activation='tanh',
      max_iter=500, random_state=0)

mlp1.fit(X_train, y_train)
print("MAE for MLP1: ", mean_absolute_error(y_test, mlp1.predict(X_test)))
mlp2.fit(X_train, y_train)
print("MAE for MLP2: ", mean_absolute_error(y_test, mlp2.predict(X_test)))
```

Code used in question 5) of **II. Programming and critical analysis** (this code is the continuation of the code used in question 4)):

```
#plots
import matplotlib.pyplot as plt

#Plot the residues (in absolute value) using two visualizations: boxplots and
histograms.

#boxplot
bp = plt.boxplot([abs(y_test - rr.predict(X_test)), abs(y_test -
      mlp1.predict(X_test)), abs(y_test - mlp2.predict(X_test))])
plt.xticks([1, 2, 3], ['Ridge', 'MLP1', 'MLP2'])
plt.ylabel('Residue')
plt.xlabel('Regressor')
plt.title('Boxplot of Residues for each regressor')
plt.show()

#histogram
plt.hist([abs(y_test - rr.predict(X_test)), abs(y_test - mlp1.predict(X_test)),
abs(y_test - mlp2.predict(X_test))], bins=40,
      label=['Ridge Regression', 'MLP1', 'MLP2'])
plt.legend()
plt.title('Histogram of Residues for each regressor')
plt.ylabel('Count')
plt.xlabel('Residue')
plt.show()
```

Code used in question 6) of **II. Programming and critical analysis** (this code is the continuation of the code used in question 4) and 5)):

```
#iterations required for MLP1 and MLP2 to converge
print('MLP1 iterations: ', mlp1.n_iter_)
print('MLP2 iterations: ', mlp2.n_iter_)
```