

## I. Pen-and-paper

1)

Consider the problem of learning a regression model from 5 univariate observations ((0.8), (1), (1.2), (1.4), (1.6)) with targets (24,20,10,13,12).

1) [5v] Consider the basis function,  $\phi_j(x) = x^j$ , for performing a 3-order polynomial regression,

$$\hat{z}(x, \mathbf{w}) = \sum_{j=0}^{3} w_j \phi_j(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3.$$

Learn the Ridge regression ( $l_2$  regularization) on the transformed data space using the closed form solution with  $\lambda=2$ .

	form solution with $\lambda = 2$ .	ns (e.g., linalg.pinv for inverse) to validate your calculus.
	11   out	$\phi: (\alpha) = \pi \dot{\phi}$
- 91 -	. 0. 8 24	$ (x_i) = (x_i) = (x_i) = (x_i) $
9 Z	1 20	
λ3.	1.2 . 10	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
પ્રદ	1.4 13 13 1	· · · · · · · · · · · · · · · · · · ·
NS	1.6 12	$\hat{z} = w^{T} \phi(x)$
. 1. (7)	$\int_{0}^{3} e^{-x} dx$	φ(x) = wo + w(x + wz n² + wz x3
X = .	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	
	1 14 14 142	163 1.16 2.56 6.096

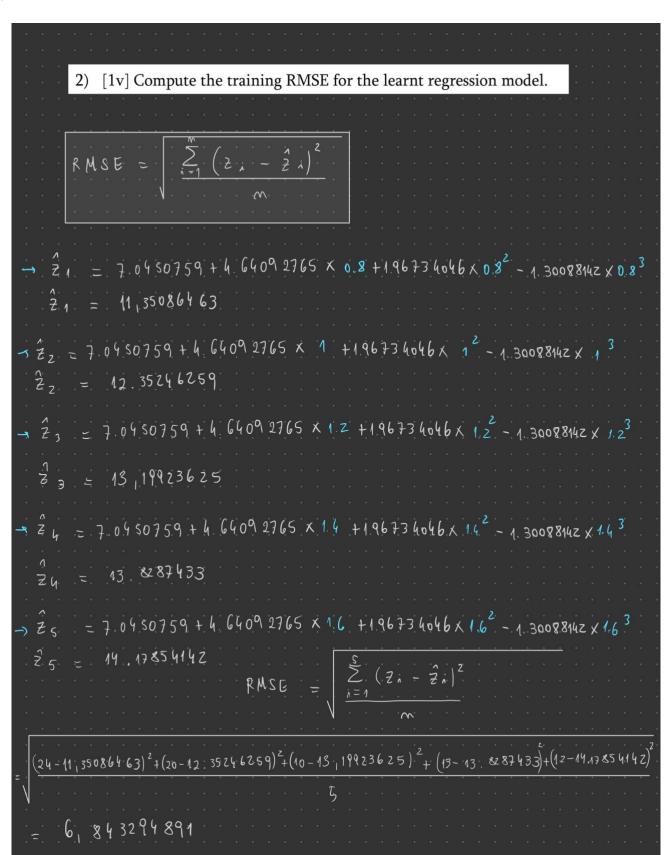


$W = ( \mathbf{D}^{T} \mathbf{D} + \lambda \mathbf{I})^{-1} \mathbf{D}^{T} \mathbf{Z}$ $\lambda = \lambda$	
$ 5^{T} 5 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0.8 & 1 & 1.2 & 1.4 & 1.6 \\ 0.64 & 1 & 1.44 & 1.96 & 2.56 \\ 0.512 & 1 & 1.728 & 2.744 & 4.096 \end{bmatrix} $	1 08 0.64 0.512 1 1 1 1 1 1.2 1.44 1.728 1 1.4 1.96 2.744 1 1.6 2.56 4.096
$= \begin{bmatrix} 5 & 6 & 7.6 & 10.08 \\ 6 & 7.6 & 10.08 & 13.8784 \\ 7.6 & 10.08 & 13.8784 & 19.68 \\ 10.08 & 13.8784 & 19.68 & 28.55488 \end{bmatrix}$	
$\lambda I = 2 \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} = 0$ $0 & 0 & 1 & 0$ $0 & 0 & 0 & 1$	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	19.68



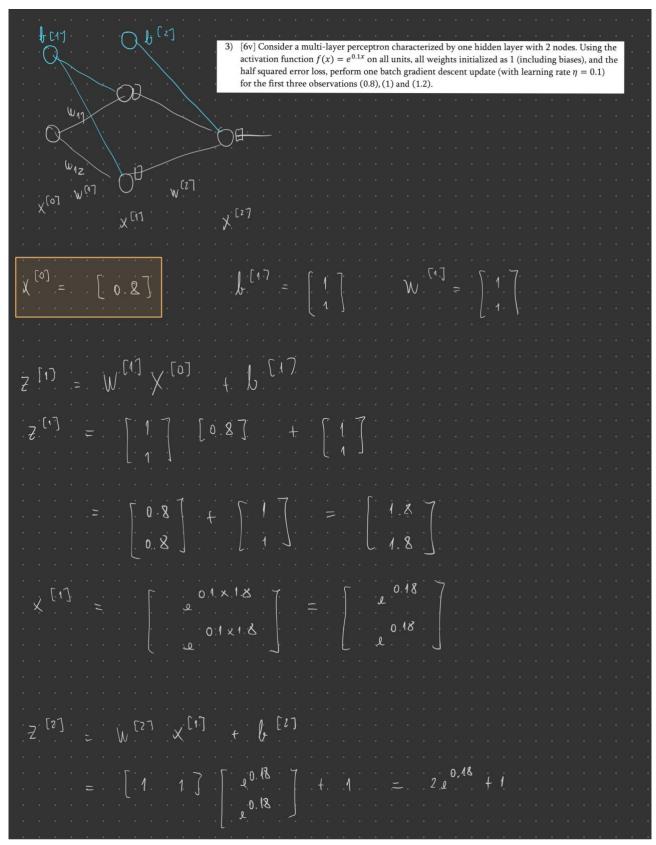
#### Homework III - Group 015

#### **2)** Answer 2

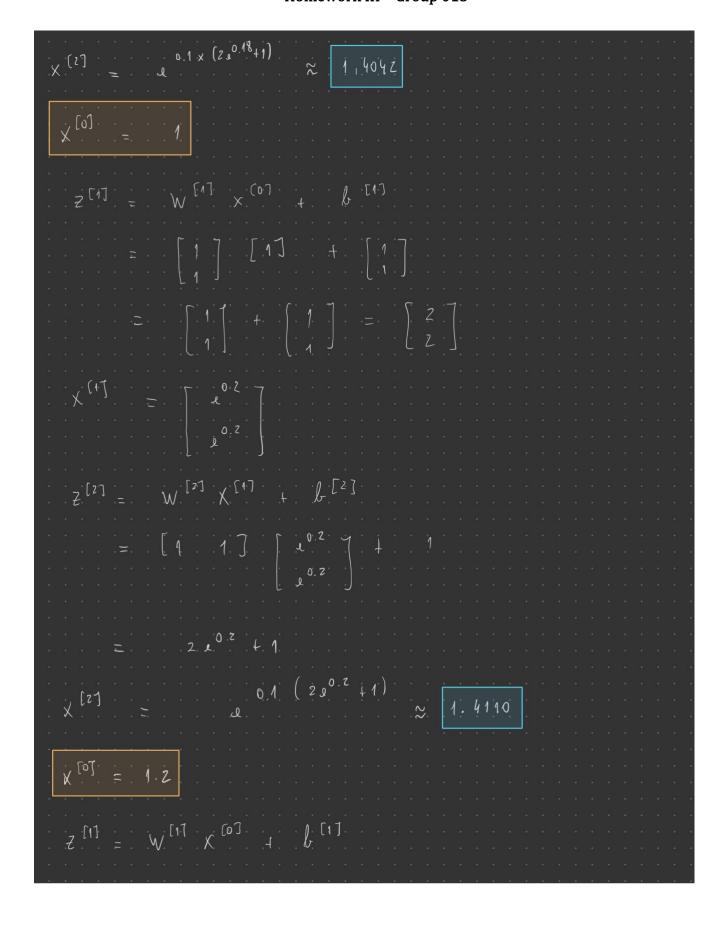


#### Homework III - Group 015

#### **3)** Answer 3









$$\begin{array}{lll}
z & = & \begin{bmatrix} 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1/2 \end{bmatrix} & + & \begin{bmatrix} 1/7 \\ 1/7 \end{bmatrix} & = & \begin{bmatrix} 2/2 \\ 2/2 \end{bmatrix} \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} & + & 1 \\
x & = & \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} &$$









$$S_{1}^{[1]} = \begin{bmatrix} -3.4728 \\ -3.4728 \end{bmatrix} \circ \begin{bmatrix} 0.1 & 2.04 \times 1.8 \\ 0.1 & 2.04 \times 1.8 \end{bmatrix}$$

$$S_{1}^{[1]} = \begin{bmatrix} -0.3799 \\ -0.3799 \end{bmatrix}$$

$$S_{2}^{[1]} = \begin{bmatrix} (W^{(2)})^{T} & S_{2}^{[2]} \end{pmatrix} \circ \begin{bmatrix} (Z_{2}^{[4]}) \\ 1 \end{bmatrix} \cdot \begin{bmatrix} -2.6229 \end{bmatrix} \circ \begin{bmatrix} 0.1 & 0.4 \times 2 \\ 0.4 & 0.4 \times 2 \end{bmatrix}$$

$$S_{2}^{[1]} = \begin{bmatrix} -2.6229 \\ -2.6229 \end{bmatrix} \circ \begin{bmatrix} 0.1 & 0.2 \\ 0.1 & 0.2 \end{bmatrix}$$

$$S_{2}^{[1]} = \begin{bmatrix} -0.3204 \\ -0.3104 \end{bmatrix}$$



$$S_{3}^{(1)} = (w^{[2]})^{T} S_{3}^{(2)} = \begin{cases} 0.1 \times 0.1 \times 2.2 \\ 0.1 \times 0.1 \times 2.2 \end{cases}$$

$$S_{3}^{(1)} = \begin{bmatrix} 1 & 1.2169 \\ -1.2169 \end{bmatrix} = \begin{bmatrix} 0.1 \times 0.22 \\ 0.1 \times 0.22 \end{bmatrix}$$

$$S_{3}^{(1)} = \begin{bmatrix} -0.4516 \\ -0.4516 \end{bmatrix} = \begin{bmatrix} -0.4516 \\ -0.4516 \end{bmatrix}$$

$$\frac{\delta \varepsilon}{\delta w^{(1)}} = \frac{2}{\delta w^{(1)}} \left( S_{3}^{(1)} - 0.3204 \\ -0.3799 \end{bmatrix} = \begin{bmatrix} 0.81 + \begin{bmatrix} -0.3204 \\ -0.3104 \end{bmatrix} \right)$$

$$+ \begin{bmatrix} -0.4516 \\ -0.4516 \end{bmatrix} = \begin{bmatrix} 0.1.2 \\ -0.4516 \end{bmatrix} =$$



$$\frac{\delta E}{\delta w^{(1)}} = \begin{bmatrix} -0.80624 \\ -0.80624 \end{bmatrix}$$

$$w^{(1)} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} - 0.1 \begin{bmatrix} -0.80624 \\ -0.80624 \end{bmatrix}$$

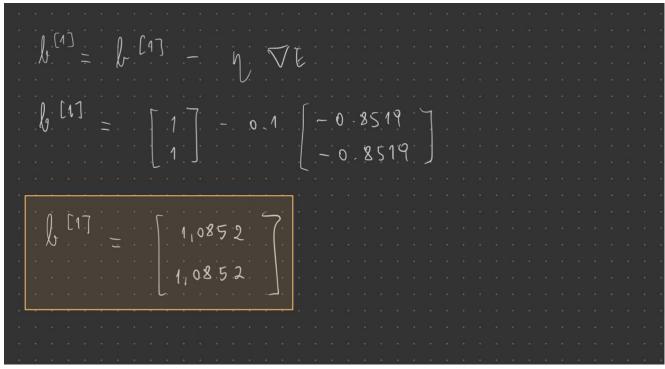
$$w^{(1)} = \begin{bmatrix} 1_{1} \\ 1_{2} \end{bmatrix} - 0.1 \begin{bmatrix} -0.80624 \\ -0.80624 \end{bmatrix}$$

$$\frac{\delta E}{\delta b^{(1)}} = \begin{bmatrix} \frac{3}{2} \\ \frac{3}{2} \end{bmatrix} \delta_{x}^{(1)}$$

$$= \begin{bmatrix} -0.3799 \\ -0.3799 \end{bmatrix} + \begin{bmatrix} -0.3204 \\ -0.3104 \end{bmatrix} + \begin{bmatrix} -0.4516 \\ -0.1516 \end{bmatrix}$$

$$= \begin{bmatrix} -0.8519 \\ -0.8519 \end{bmatrix}$$





II. Programming and critical analysis

#### **4)** Answer 4

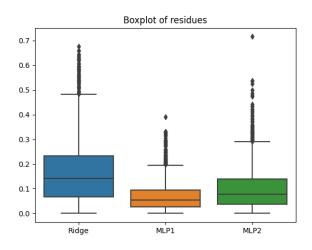
Mean Absolute Error Ridge Linear Regression: 0.162829976437694

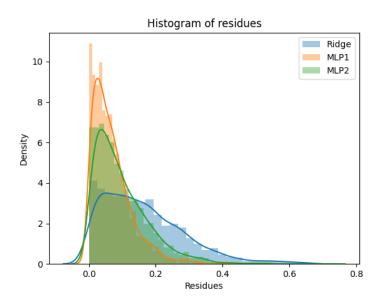
Mean Absolute Error MLP1: 0.0680414073796843

Mean Absolute Error MLP2: 0.0978071820387748

#### **5)** Answer 5







#### **6)** Answer 6

MLP1 iterations to converge: 452 MLP2 iterations to converge: 77

#### **7)** Answer 7

What is motivating the difference between the number of iterations of both MLPs is the early stopping. The fact that the first MLP is parameterized with early stopping helps fighting overfitting. When this parameter is set to true, it will automatically set aside 10% of training data as validation and terminate when validation score is not improving by at least a certain number of consecutive epochs. By doing this, we prevent the algorithm from getting too accustomed to the training data and, therefore, it needs more iterations to converge, whereas when this parameter is set to false, the training



#### Homework III - Group 015

stops when the training loss does not improve by more than a certain number of consecutive passes over the training set. For these reasons, the second MLP converges much faster.

Regarding the observed performance differences between the MLPs, the one with early stopping demonstrates lower average residues and a lower Mean Absolute Error (MAE), which could be due to the fact that, as we fight overfitting, this trained neural network is better "prepared" when it comes to predicting the outcome of the testing data. On the other hand, the second MLP shows higher average residues and a higher MAE which could be a direct consequence of overfitting. By not parameterizing the second MLP with early stopping, this model fits to the training data to an extent that, compared to the first one, damages the generalization performance.

#### III. APPENDIX

```
from sklearn.linear_model import LinearRegression, Ridge, Lasso
import pandas as pd
from scipy.io.arff import loadarff
from sklearn.model selection import train test split
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.neural network import MLPRegressor
from sklearn import metrics, datasets
data = loadarff('kin8nm.arff')
df = pd.DataFrame(data[0])
X = df.drop('y', axis=1)
y = df['y']
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.30, random_state = 0)
ridge = Ridge(alpha = 0.1)
ridge.fit(X_train, y_train)
y_pred_Ridge = ridge.predict(X_test)
print("Mean Absolute Error Ridge Linear Regression:", metrics.mean_absolute_error(y_test,
y_pred_Ridge))
mlp1 = MLPRegressor(hidden_layer_sizes = (10, 10), activation = "tanh", max_iter = 500, random_state
= 0, early_stopping = True)
mlp1.fit(X_train.values, y_train)
y_pred_mlp1 = mlp1.predict(X_test.values)
print("Mean Absolute Error MLP1:", metrics.mean_absolute_error(y_test, y_pred_mlp1))
```



```
mlp2 = MLPRegressor(hidden_layer_sizes = (10, 10), activation = "tanh", max_iter=500, random_state =
0, early_stopping = False, verbose = True)
mlp2.fit(X_train.values, y_train)
y_pred_mlp2 = mlp2.predict(X_test.values)
print("Mean Absolute Error MLP2:", metrics.mean_absolute_error(y_test, y_pred_mlp2))
ridgeResidues = abs(y_test - y_pred_Ridge)
MLP1Residues = abs(y_test - y_pred_mlp1)
MLP2Residues = abs(y_test - y_pred_mlp2)
residues = pd.DataFrame({"Ridge": ridgeResidues, "MLP1": MLP1Residues, "MLP2": MLP2Residues})
sns.boxplot(data = residues)
plt.title("Boxplot of residues")
plt.savefig("boxplots.png")
plt.show()
sns.distplot(residues["Ridge"], hist = True, label = "Ridge")
sns.distplot(residues["MLP1"], hist = True, label = "MLP1")
sns.distplot(residues["MLP2"], hist = True, label = "MLP2")
plt.title("Histogram of residues")
plt.legend()
plt.xlabel("Residues")
plt.savefig("histograms.png")
plt.show()
print("MLP1 iterations to converge:", mlp1.n iter )
print("MLP2 iterations to converge:", mlp2.n_iter_)
if mlp1.n_iter_ < mlp1.max_iter:</pre>
    print("MLP1 converged")
else:
    print("MLP1 did not converge")
if mlp2.n_iter_ < mlp2.max_iter:</pre>
    print("MLP2 converged")
else:
    print("MLP2 did not converge")
```