### Homework III - Group 35

(ist1100032, ist1100070)

### I. Pen-and-paper

1) (1) a -  $\phi_{1}(x) = \exp\left(-\frac{\|x - c_{1}\|^{2}}{2}\right)$ 8= (0,8;0,6;0,3;0,3) \ \{\begin{pmatrix} \( \begin{pmatrix} \( \cdot \) \\ \( \cdo \) \\ \( \cdot \) \\ \( \cdo \) \\\ \( \cdo \) \\\ \( \cdo \) \\\ \( \cdo \) \\\ \( \cdo \) \\ \( \cdo \) \\\ \( \cdo \) \\\ \( \cdo \) \\\ \( \cdo \) \\\ \( \  $C_{1}=\begin{pmatrix} 0 \\ 0 \end{pmatrix}$   $C_{2}=\begin{pmatrix} 1 \\ -1 \end{pmatrix}$   $C_{3}=\begin{pmatrix} -1 \\ 1 \end{pmatrix}$ Ridge: W=(xTx+ \L)'xTz / \=0,1  $\phi_1({0,7 \atop -0,3}) = 0.74826$   $\phi_2({0,7 \atop -0,3}) = 0.74826$  $\phi_1\left(\begin{array}{c} 0.19\\ 0.15 \end{array}\right) = 0.81465 \qquad \phi_2\left(\begin{array}{c} 0.14\\ 0.15 \end{array}\right) = 0.27117$  $\Phi_{1}(\frac{-0.2}{0.8}) = 0.71177$   $\Phi_{2}(\frac{-0.2}{0.8}) = 0.09633$  $\phi_1(\frac{-0.4}{0.13}) = 0.88250$   $\phi_2(\frac{-0.4}{0.13}) = 0.16122$ \$\left(\frac{0}{-0.3}\right) = 0,10127  $\phi_3(0,4) = 0,33121$ \$ 3 ( -0/2 ) = 0/7/177 Φ3(-0,4)=0,65377 0,74826 0,74826 0,10127  $X = \begin{cases} 1 & 0.81465 & 0.27117 & 0.33121 \\ 1 & 0.771177 & 0.09633 & 0.771177 \end{cases}$ 1 0,88250 0,16122 0,65377



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$$X^{T}X = \begin{bmatrix} 4 & 3,15718 & 1,27698 & 4,79802 \\ 3,15718 & 2,50897 & 0,99165 & 1,42916 \\ 1,27698 & 0,99165 & 0,66670 & 0,33955 \\ 1,79802 & 4,42916 & 0,38955 & 1,05399 \end{bmatrix}$$

$$X^{T}X + \lambda I = \begin{bmatrix} 4,1 & 3,15718 & 1,27698 & 4,79802 \\ 3,15718 & 2,60897 & 0,99165 & 1,42916 \\ 1,27698 & 0,99165 & 0,76320 & 0,33955 \\ 4,79302 & 1,42916 & 0,33955 & 1,15399 \end{bmatrix}$$

$$(X^{T}X + \lambda I)^{-1} = \begin{bmatrix} 4,54826 & -3,79682 & -1,86117 & -1,86155 \\ -3,73682 & 5,78285 & -0,28543 & 1,26432 \\ -1,86117 & -0,88543 & 4,33276 & 2,72156 \\ -1,86155 & -126432 & 2,72156 & 4,53204 \end{bmatrix}$$

$$(X^{T}X + \lambda I)^{-1}X^{T} = \begin{bmatrix} 0,4105 & 0,35022 & 0,35575 & -0,30185 \\ -0,09064 & 0,43823 & -0,50615 & -0,43610 & -0,16477 \\ -0,3122 & -0,65246 & 0,72647 & 0,42436 \end{bmatrix}$$

$$(X^{T}X + \lambda I)^{-1}X^{T}J = [0,33914 0,19945 0,40096 -0,29600]$$



(ist1100032, ist1100070)

#### Código Python auxiliar:

1a)



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```
# Regularization parameter (λ)
   alpha = 0.1
   # Define the RBF centers
   centers = [(0, 0), (1, -1), (-1, 1)]
   # Initialize an empty array for the transformed data
   X_transformed = np.zeros((len(column1), len(centers)))
   for j, center in enumerate(centers):
       for i in range(len(column1)):
           x = np.array([column1[i], column2[i]])
           c = np.array(center)
           X_{\text{transformed}[i, j]} = \text{np.exp(-np.linalg.norm}(x - c)**2 / 2)
   # Add a column of 1s for the bias term
   bias_column = np.ones((len(column1), 1))
   X_transformed = np.hstack((bias_column, X_transformed))
   print(X_transformed)
[[1.
             0.74826357 0.74826357 0.10126646]
[1.
             0.81464732 0.27117254 0.33121088]
             0.71177032 0.09632764 0.71177032]
 [1.
             0.8824969 0.16121764 0.65376979]]
 [1.
```

```
np.matmul(X_transformed.T, X_transformed)

array([[4. , 3.15717811, 1.27698138, 1.79801745],
        [3.15717811, 2.50896639, 0.99164557, 1.42916086],
        [1.27698138, 0.99164557, 0.66870305, 0.33955168],
        [1.79801745, 1.42916086, 0.33955168, 1.05398747]])
```

Learn the Ridge regression (12 regularization) using the closed solution



inv = np.linalg.pinv(np.matmul(X\_transformed.T, X\_transformed) + alpha \* np.identity(4))
inv

array([[ 4.54826202, -3.77681832, -1.86116983, -1.86155421],
 [-3.77681832, 5.98284561, -0.88542926, -1.26432443],
 [-1.86116983, -0.88542926, 4.33275508, 2.72155678],
 [-1.86155421, -1.26432443, 2.72155678, 4.53204296]])

```
W_ridge = np.matmul(moore_penrose, y)
W_ridge
array([ 0.33914267,  0.19945264,  0.40096085, -0.29599936])
```

1b)

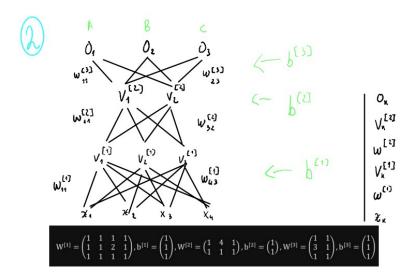
```
y_pred = np.dot(X_transformed, W_ridge)

rmse = np.sqrt(np.mean((y - y_pred)**2))

print("RMSE:", rmse)

RMSE: 0.06508238153393446
```

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$$\chi^{(0)(1)}_{=\chi_{2}} = \begin{cases} 1 \\ 1 \\ 1 \end{cases} \quad \hat{Z}_{1} = B$$

$$\chi^{(0)(1)}_{=\chi_{2}} = \begin{cases} 1 \\ 0 \\ -1 \end{cases} \quad \hat{Z}_{2} = A$$

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For ward propagation:  

$$x^{(0)} = x_{1} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\chi^{c_{1}}_{=}^{(1)} = \text{activation}(z^{(1)(1)}) = \begin{bmatrix} 0.46212\\ 0.76159\\ 0.46212 \end{bmatrix}$$

$$Z^{[2](1)} = w^{[2]} \cdot \chi^{[1](1)} + b^{[2]} = \begin{bmatrix} 1 & 4 & 1 \\ 1 & 1 & 4 \end{bmatrix} \cdot \begin{bmatrix} 0.462 & 1 & 2 \\ 0.761 & 5 & 9 \\ 0.462 & 1 & 2 \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 4.8706 & 1 \\ 2.68582 \end{bmatrix}$$

$$\times \left[ \begin{array}{c} 2 & 3^{(1)} \\ = & \text{activation} \left( z^{(1)(1)} \right) = \begin{bmatrix} 0.45048 \\ -0.57642 \end{bmatrix} \\ 2x1 \end{array} \right]$$

$$Z = W^{[3]} \times X^{[2](1)} + b^{[3]} = \begin{bmatrix} 1 & 1 \\ 3 & 1 \\ 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 0.45068 \\ -0.57642 \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0.87406 \\ 1.77502 \\ 0.87406 \end{bmatrix}$$

$$\times \begin{bmatrix} 3 & 3 & (1) \\ & = & \text{activation} & (2^{(3)})^{(1)} \end{bmatrix} = \begin{bmatrix} -0.91390 \\ -0.80493 \\ -0.91590 \end{bmatrix}$$
3×1

input 
$$\chi^{(0)}(z) = \chi_{\underline{L}} = \begin{bmatrix} 1 \\ 8 \\ -1 \end{bmatrix}$$

$$Z^{[1](2)} = W^{[1]} \cdot X^{[0](2)} + b^{[1]} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \\ 0 \\ -1 \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$= \chi^{c_{1}}_{3}(2) = Activation (Z^{(1)(2)}) = \begin{bmatrix} -0.90515 \\ -0.90515 \\ -0.90515 \end{bmatrix}$$

$$= 3 \times 1$$

$$Z^{[2](2)} = W^{[2]} \cdot \chi^{[1](2)} + b^{[2]} = \begin{bmatrix} 1 & 4 & 1 \\ 1 & 4 & 4 \end{bmatrix} \cdot \begin{bmatrix} -0.90515 \\ -0.90515 \\ -0.90515 \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -4.43089 \\ -1.71544 \end{bmatrix}$$

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$$\times^{[2](2)} = \text{activation}(Z^{(1)(1)}) = \begin{bmatrix} -0.99856 \\ -0.99343 \end{bmatrix}$$

$$Z^{[3](2)} = W^{[3]} \cdot \chi^{[2](2)} + b^{[3]} = \begin{bmatrix} 1 & 1 \\ 3 & 1 \\ 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} -0.89056 \\ -0.90343 \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -0.90299 \\ -2.99212 \\ -0.90299 \end{bmatrix}$$

$$\chi^{[3](2)} = \text{activation}(z^{(3)(1)}) = \begin{bmatrix} -0.98652\\ -0.94816\\ -0.98632 \end{bmatrix}$$
3×1

# Backpropagation

derive the activation function:

$$\frac{dk(x)}{dx} = \frac{d \tanh(0.5\%-2)}{d \%} = 5ech^{2}(0.5\%-2)\cdot0.5$$

$$\frac{9^{x_{t,3}}}{9 E(f' x_{t;3})} = x_{t;1} - f$$

$$\frac{\partial \mathbf{z}^{[i]}(\mathbf{W}^{[i]}, \mathbf{b}^{[i]}, \mathbf{x}^{[i-1]})}{\partial \mathbf{W}^{[i]}} = \mathbf{x}^{[i-1]}$$

$$\frac{\partial \mathbf{z}^{[i]}(\mathbf{W}^{[i]}, \mathbf{b}^{[i]}, \mathbf{x}^{[i-1]})}{\partial \mathbf{b}^{[i]}} = \mathbf{1}$$

$$\frac{\partial \mathbf{z}^{[i]}(\mathbf{W}^{[i]}, \mathbf{b}^{[i]}, \mathbf{x}^{[i-1]})}{\partial \mathbf{x}^{[i-1]}} = \mathbf{W}^{[i]}$$

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# cálculo dos 8 ~ r squared er ror 1055

# 8<sup>13</sup> (last layer)

$$S^{[3](1)} = \frac{\partial E}{\partial x^{[3](1)}} O \frac{\partial x^{[3](1)}}{\partial z^{[3](1)}} = (x^{[3](1)} - (x^{[3](1)}) \circ \frac{\partial (\tanh(0.5 \cdot z^{(3)(1)} - z))}{\partial z^{[3](1)}} =$$

$$= (x^{[3](1)} - (x^{[3](1)}) \circ (x^{[3]$$

$$S^{[3](2)} = \frac{\partial E}{\partial x^{[3](2)}} - \frac{\partial Z^{[3](2)}}{\partial z^{[3](2)}} = (x^{[3](2)} - (x^{[2](2)}) \circ \frac{\partial (\tanh(0.5 z^{[3](2)} - 2)}{\partial z^{[3](2)}} =$$

$$= (x^{[3](1)} - (x^{[1]}) \circ (x^{[3](2)} - (x^{[3](2)}) \circ (x^{[3](2)} - (x^{[3](2)})) = \begin{bmatrix} -2.65 \text{ s} \times 10^{-2} \\ 3.369 \times 10^{-6} \\ 1.804 \times 10^{-6} \end{bmatrix}$$

$$\frac{\delta}{\delta} = \left(\frac{\partial z^{[3](1)}}{\partial x^{[2](1)}}\right)^{T} \cdot \delta^{[3](1)} \circ \frac{\partial x^{[2](1)}}{\partial z^{[2](1)}} = (w^{[3]})^{T} \cdot \delta^{[3](1)} \circ (0.5 \cdot 5ech^{2}(0.5 Z^{[2](1)})) = \left[-0.37448 -0.10156\right]$$

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$$S[1](2) = \left(\frac{dz^{[2](2)}}{dx^{[1](2)}}\right)^{T} \cdot S^{[2](2)} \circ \frac{dx^{[1](2)}}{dz^{[1]}} = (w^{[2]})^{T} \cdot S^{[2](2)} \circ (0.5 \cdot 5ech^{2}(0.5 Z^{[1](2)}) = \left[\frac{-1.666 \times 10^{-5}}{-1.606 \times 10^{-5}}\right]$$

Updates

$$w^{Li3} = w^{Li3} - \gamma \cdot \frac{\partial E}{\partial w^{Li3}} \qquad \frac{\partial E}{\partial w^{Li3}} = \sum_{j=1}^{N} \frac{\partial E}{\partial x^{Li3(j)}} \cdot \frac{\partial x^{Li3(j)}}{\partial w^{Li3(j)}}^{T}$$

$$b^{Li3} = b^{Li3} - \gamma \cdot \frac{\partial E}{\partial b^{Li3}} \qquad \frac{\partial E}{\partial b^{Li3}} = \sum_{j=1}^{N} S^{Ci3(j)}$$

$$\frac{\text{Mive} | 3}{\text{w}^{133}} = w^{133} - y \cdot \frac{JE}{Jw^{133}} = \begin{bmatrix} 0.98703 & 0.98769 \\ 3.01631 & 0.98169 \\ 0.98971 & 1.00041 \end{bmatrix}$$

$$\frac{\partial VX}{\partial w^{(3)}} = \begin{cases} \left[33(1) \cdot \left(\chi^{(2)}(1)\right)^{T} + \left(33(2) \cdot \left(\chi^{(2)}(2)\right)^{T} = \begin{bmatrix} 0.02964 & 0.022516 \\ -0.10314 & 0.19314 \\ 0.00287 & -0.00408 \end{bmatrix} \right]$$

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$$\frac{AUX}{\frac{1}{2}b^{[3]}} = \begin{cases} E^{[3](1)} + \int_{0.00696}^{[3](2)} = \begin{bmatrix} -0.01982 \\ -0.31773 \\ 0.00696 \end{bmatrix}$$

# nível 2

$$\mathbf{w}^{L^{2}J} = \mathbf{w}^{L^{2}J} - \mathbf{y} \cdot \frac{\mathbf{j}E}{\mathbf{j}\mathbf{w}^{L^{2}J}} = \begin{bmatrix} 1.01730 & 4.02851 & 1.01730 \\ 1.00467 & 1.00772 & 1.00468 \end{bmatrix}$$

$$\mathbf{w}^{L^{2}J} = \mathbf{k}^{L^{2}J(1)} \cdot \mathbf{k}^{L^{2}J(1)} \cdot \mathbf{k}^{L^{2}J(1)} \cdot \mathbf{k}^{L^{2}J(2)} \cdot \mathbf{k}^{L^{2}J(2)} \cdot \mathbf{k}^{L^{2}J(2)} = \begin{bmatrix} -0.17304 & -0.28519 & -0.17304 \\ -0.04677 & -0.07719 & -0.04677 \end{bmatrix}$$

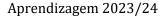
• 
$$b^{(2)} = b^{(2)} - y \frac{\partial E}{\partial b^{(2)}} = \begin{bmatrix} 1.03743 \\ 1.01017 \end{bmatrix}$$

$$\frac{AUX}{\int b^{(2)}} = 8^{(2)(1)} + 8^{(2)(2)} = \begin{bmatrix} -0.37449 \\ -0.10173 \end{bmatrix}$$

$$= w^{[1]} - \sqrt{\frac{JE}{Ju^{[1]}}} = \begin{vmatrix} 1.01872 & 1.01872 & 1.01872 & 1.01872 & 1.01872 & 1.01872 & 1.03338 & 1.03338 & 1.03338 & 1.03338 & 1.01872 &$$

$$b^{[1]} = b^{[1]} - y \frac{JE}{Jb^{[1]}} = \begin{bmatrix} 1.01872\\ 1.03359\\ 1.01872 \end{bmatrix}$$

$$\frac{AUX}{\int b^{(1)}} = \begin{cases} \sum_{i=1}^{L^{1/3}(1)} + \sum_{i=1}^{L^{1/3}(2)} = \begin{bmatrix} -0.18720 \\ -0.33389 \\ -0.18721 \end{bmatrix}$$





Código python auxiliar:

```
learning_rate = 0.1
W1 = np.array([[1, 1, 1, 1],
                [1, 1, 2, 1],
                [1, 1, 1, 1]])
b1 = np.array([[1],
                [1]])
W2 = np.array([[1, 4, 1],
                [1, 1, 1]])
b2 = np.array([[1],
                [1]])
W3 = np.array([[1, 1],
                [3, 1],
                [1, 1]])
b3 = np.array([[1],
                [1],
                [1]])
```



# **Forward Propagation**

Para o input X0\_1 (x1 do enunciado) -> \_1 indica isso

```
Z1_1 = np.matmul(W1, X0_1) + b1
Z1_1

array([[5],
       [6],
       [5]])

X1_1 = activation_function(Z1_1)
    X1_1

array([[0.46211716],
       [0.76159416],
       [0.46211716]])
```



# Para o input X0\_2 (x2 do enunciado) \_2 indica isso



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# Backpropagation

derived activation function

```
def derived_actication_function(x):
    return (1 / (np.cosh(0.5 * x - 2) ** 2)) * 0.5
```

```
delta3_1 = np.multiply((X3_1 - t1), derived_actication_function(Z3_1))
delta3_1

array([[ 0.00677537],
        [-0.31773455],
        [ 0.00677537]])

delta3_2 = np.multiply((X3_2 - t2), derived_actication_function(Z3_2))
        delta3_2

array([[-2.65961421e-02],
        [ 3.36962051e-06],
        [ 1.80462886e-04]])
```



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```
dE_db3 = (delta3_1 + delta3_2)
dE_db3

array([[-0.01982077],
        [-0.31773118],
        [ 0.00695584]])

b3_new = b3 - (learning_rate * dE_db3)
b3_new

array([[1.00198208],
        [1.03177312],
        [0.99930442]])
```



```
Nível 2

dE_dW2 = (delta2_1 * X1_1.T) + (delta2_2 * X1_2.T)
dE_dW2

array([[-0.17304435, -0.28519324, -0.17304435],
        [-0.04677506, -0.07718926, -0.04677506]])

W2_new = W2 - (learning_rate * dE_dW2)
W2_new

array([[1.01730444, 4.02851932, 1.01730444],
        [1.00467751, 1.00771893, 1.00467751]])
```



```
dE_db1 = (delta1_1 + delta1_2)
dE_db1

array([[-0.18720702],
        [-0.33589165],
        [-0.18720702]])

b1_new = b1 - (learning_rate * dE_db1)
b1_new

array([[1.0187207],
        [1.03358917],
        [1.0187207]])
```



#### II. Programming and critical analysis

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.neural_network import MLPRegressor
from sklearn.metrics import mean_absolute_error
from sklearn.metrics import mean_squared_error

file_path = "winequality-red.csv"

df = pd.read_csv(file_path, delimiter=';')

X = df.drop('quality', axis=1)
y = df['quality']

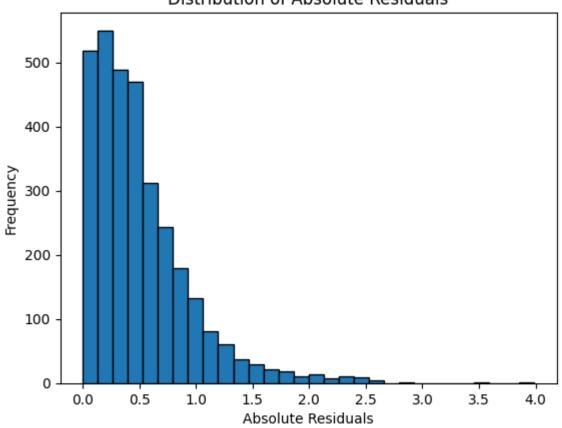
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=0)
```

```
num runs = 10
random_states = range(1, num_runs + 1)
residuals = []
mae_original = []
mae_values_rounded_bounded = []
for random_state in random_states:
   mlp = MLPRegressor(hidden_layer_sizes=(10, 10), activation='relu', early_stopping=True, validation_fraction=0.2, random_state=random_state)
   mlp.fit(X_train, y_train)
   y_pred = mlp.predict(X_test)
    residuals.extend(np.abs(y_test - y_pred))
   # Calculate MAE for original predictions (variable) y_test: Any
   mae_original.append(mean_absolute_error(y_test, y_pred))
   y_pred_rounded = np.round(y_pred)
   y_pred_rounded_bounded = np.clip(y_pred_rounded, 1, 10)
    mae_rounded_bounded = mean_absolute_error(y_test, y_pred_rounded_bounded)
    mae_values_rounded_bounded.append(mae_rounded_bounded)
plt.hist(residuals, bins=30, edgecolor='k')
plt.xlabel('Absolute Residuals')
plt.ylabel('Frequency')
plt.title('Distribution of Absolute Residuals')
plt.show()
```



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#### Distribution of Absolute Residuals



```
# Calculate the average MAE for original predictions and rounded predictions
avg_mae_original = np.mean(mae_original)
avg_mae_rounded_bounded = np.mean(mae_values_rounded_bounded)

print(f"Average MAE without rounding and bounding: {avg_mae_original:.4f}")
print(f"Average MAE with rounding and bounding: {avg_mae_rounded_bounded:.4f}")

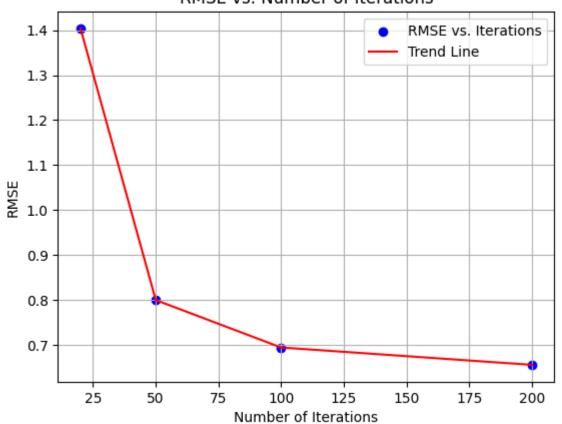
Average MAE without rounding and bounding: 0.5097
Average MAE with rounding and bounding: 0.4388
```



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```
iteration_settings = [20, 50, 100, 200]
rmse_results = []
for iterations in iteration_settings:
    aux_rmse_results = []
    for random_state in random_states:
        mlp = MLPRegressor(hidden_layer_sizes=(10, 10), activation='relu', max_iter=iterations, validation_fraction=0.2, random_state=random_state)
        mlp.fit(X_train, y_train)
        y_pred = mlp.predict(X_test)
        rmse = np.sqrt(mean_squared_error(y_test, y_pred))
        aux_rmse_results.append(rmse)
    rmse_results.append(np.mean(aux_rmse_results))
plt.scatter(iteration_settings, rmse_results, marker='o', color='b', label='RMSE vs. Iterations')
plt.plot(iteration_settings, rmse_results, linestyle='-', color='r', label='Trend Line')
plt.xlabel('Number of Iterations')
plt.ylabel('RMSE')
plt.title('RMSE vs. Number of Iterations')
plt.grid(True)
plt.legend()
plt.show()
```







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4) The results show a clear trend as the number of iterations increases, the RMSE generally decreases, indicating better model performance.

Early stopping helps prevent overfitting by stopping training when the validation error starts to increase, preventing the model from over-optimizing on the training data, leading to better generalization. It can also save trining time which is most relevant in bigger models. On the other hand, early stopping can worsen performance when a model stops learning before it has converged to the optimal solution (global minimum of the loss function), particularly relevant if the chosen number of iterations is too small, leading to underfitting, where the model lacks the complexity to capture the underlying patterns in the data effectively. If the validation set is not representative of the test data or is too small, early stopping may also stop training prematurely or continue training unnecessarily, leading to suboptimal performance.

**END**