# ML-HW4-Q1\_Q4\_v2

February 19, 2025

### 1 Machine Learning - Homework 4

Author: Shivani Tayade, Sravya Bhaskara

70

usa

### 1.0.1 Linear Regression with PyTorch on the Auto MPG Dataset

```
[3]: import seaborn as sns
     import pandas as pd
     import matplotlib.pyplot as plt
     import numpy as np
     import matplotlib.pyplot as plt
     from sklearn.preprocessing import StandardScaler
     from sklearn.model_selection import train_test_split
     from sklearn.metrics import mean_squared_error, r2_score
[4]: # Load dataset
     df = sns.load_dataset('mpg')
     df
[4]:
                cylinders
                            displacement
                                           horsepower
                                                        weight
                                                                acceleration
           mpg
          18.0
                         8
                                    307.0
                                                          3504
                                                                         12.0
     0
                                                 130.0
                         8
     1
          15.0
                                    350.0
                                                 165.0
                                                          3693
                                                                         11.5
     2
          18.0
                         8
                                                          3436
                                                                         11.0
                                    318.0
                                                 150.0
     3
                         8
          16.0
                                    304.0
                                                 150.0
                                                          3433
                                                                         12.0
     4
          17.0
                         8
                                    302.0
                                                 140.0
                                                          3449
                                                                         10.5
     393
         27.0
                         4
                                    140.0
                                                  86.0
                                                          2790
                                                                         15.6
     394 44.0
                         4
                                     97.0
                                                  52.0
                                                          2130
                                                                         24.6
                                                                         11.6
     395 32.0
                         4
                                    135.0
                                                  84.0
                                                          2295
     396 28.0
                         4
                                    120.0
                                                  79.0
                                                          2625
                                                                         18.6
                         4
                                    119.0
                                                  82.0
     397
         31.0
                                                          2720
                                                                         19.4
          model_year
                       origin
                                                      name
     0
                               chevrolet chevelle malibu
                  70
                          usa
                  70
     1
                                        buick skylark 320
                          usa
     2
                  70
                          usa
                                       plymouth satellite
     3
                   70
                                            amc rebel sst
                          usa
```

ford torino

```
393
              82
                                      ford mustang gl
                      usa
394
              82
                  europe
                                             vw pickup
395
              82
                                        dodge rampage
                      usa
396
              82
                                          ford ranger
                      usa
397
              82
                                            chevy s-10
                      usa
```

[398 rows x 9 columns]

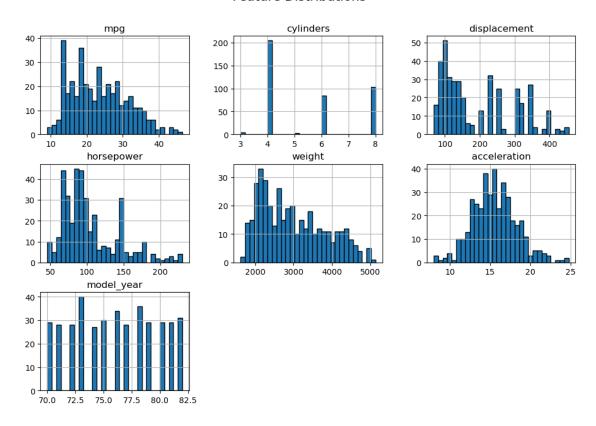
```
[5]: df.describe()
```

```
[5]:
                          cylinders
                                      displacement
                                                     horsepower
                                                                       weight
                    mpg
     count
            398.000000
                         398.000000
                                        398.000000
                                                     392.000000
                                                                   398.000000
                           5.454774
                                                     104.469388
                                                                  2970.424623
     mean
             23.514573
                                        193.425879
     std
              7.815984
                           1.701004
                                        104.269838
                                                      38.491160
                                                                   846.841774
     min
              9.000000
                           3.000000
                                         68.000000
                                                      46.000000
                                                                  1613.000000
     25%
                           4.000000
                                        104.250000
                                                      75.000000
                                                                 2223.750000
             17.500000
     50%
             23.000000
                           4.000000
                                        148.500000
                                                      93.500000
                                                                  2803.500000
     75%
                           8.000000
                                        262.000000
                                                     126.000000
             29.000000
                                                                  3608.000000
     max
             46.600000
                           8.000000
                                        455.000000
                                                     230.000000
                                                                 5140.000000
            acceleration
                           model_year
              398.000000
                           398.000000
     count
                15.568090
                            76.010050
     mean
     std
                2.757689
                             3.697627
     min
                8.000000
                            70.000000
     25%
                13.825000
                            73.000000
     50%
                15.500000
                            76.000000
     75%
                17.175000
                            79.00000
                            82.000000
     max
                24.800000
```

```
[6]: plt.figure(figsize=(12, 8))
    df.hist(figsize=(12, 8), bins=30, edgecolor='black')
    plt.suptitle("Feature Distributions", fontsize=16)
    plt.show()
```

<Figure size 1200x800 with 0 Axes>

### Feature Distributions



### [7]: df.isnull().sum()

[7]: mpg 0 cylinders 0 displacement 0 horsepower 6 weight 0 acceleration 0 model\_year 0 origin 0 namedtype: int64

There are null values in the data for variable horsepower

```
[9]: # Drop rows with missing values
df_drop = df.dropna()
print("Shape after dropping missing values:", df_drop.shape)
```

```
Shape after dropping missing values: (392, 9)
```

```
[10]: # Approach 2: Impute missing values
      # For numerical columns, we can impute using the mean
      numerical_cols = df.select_dtypes(include=['float64', 'int64']).columns
      df_imputed = df.copy()
      for col in numerical_cols:
          if df_imputed[col].isnull().sum() > 0:
              mean_value = df_imputed[col].mean()
              df_imputed[col].fillna(mean_value, inplace=True)
[11]: # For categorical columns, we might choose the mode
      categorical_cols = df.select_dtypes(include=['object', 'category']).columns
      for col in categorical_cols:
          if df imputed[col].isnull().sum() > 0:
              mode_value = df_imputed[col].mode()[0]
              df_imputed[col].fillna(mode_value, inplace=True)
      print("Missing values after imputation:")
      print(df_imputed.isnull().sum())
     Missing values after imputation:
     mpg
                     0
     cylinders
     displacement
                     0
     horsepower
                     0
                     0
     weight
     acceleration
                     0
     model_year
                     0
     origin
     name
     dtype: int64
[12]: df['horsepower'].describe()
[12]: count
               392.000000
     mean
               104.469388
      std
                38.491160
     min
                46.000000
      25%
                75.000000
      50%
                93.500000
      75%
               126.000000
               230.000000
      max
      Name: horsepower, dtype: float64
[13]: df_imputed['horsepower'].describe()
```

```
[13]: count
                398.000000
      mean
                104.469388
      std
                 38.199187
      min
                 46.000000
      25%
                 76.000000
      50%
                 95.000000
      75%
                125.000000
      max
                230.000000
      Name: horsepower, dtype: float64
[14]: df_imputed1 = df_imputed.drop(columns=['name','origin','model_year'])
      df_imputed1
Γ14]:
                  cylinders
                             displacement
                                            horsepower
                                                         weight
                                                                  acceleration
            mpg
      0
           18.0
                          8
                                     307.0
                                                  130.0
                                                            3504
                                                                           12.0
      1
           15.0
                          8
                                                                           11.5
                                     350.0
                                                  165.0
                                                            3693
      2
           18.0
                          8
                                     318.0
                                                  150.0
                                                            3436
                                                                           11.0
      3
                          8
                                                                           12.0
           16.0
                                     304.0
                                                  150.0
                                                            3433
      4
           17.0
                          8
                                     302.0
                                                  140.0
                                                            3449
                                                                           10.5
      393
           27.0
                          4
                                                            2790
                                                                           15.6
                                     140.0
                                                   86.0
           44.0
      394
                          4
                                      97.0
                                                   52.0
                                                            2130
                                                                           24.6
      395
           32.0
                          4
                                                   84.0
                                     135.0
                                                            2295
                                                                           11.6
                          4
      396
           28.0
                                     120.0
                                                   79.0
                                                            2625
                                                                           18.6
      397
           31.0
                                     119.0
                                                   82.0
                                                            2720
                                                                           19.4
      [398 rows x 6 columns]
[15]: df_imputed1.corr()
[15]:
                                cylinders
                                            displacement
                                                                          weight
                                                          horsepower
                          mpg
                                -0.775396
                                               -0.804203
                                                            -0.771437 -0.831741
      mpg
                     1.000000
      cylinders
                    -0.775396
                                 1.000000
                                                0.950721
                                                             0.838939
                                                                       0.896017
      displacement -0.804203
                                                1.000000
                                 0.950721
                                                             0.893646
                                                                       0.932824
                    -0.771437
      horsepower
                                 0.838939
                                                0.893646
                                                             1.000000
                                                                       0.860574
      weight
                    -0.831741
                                 0.896017
                                                0.932824
                                                             0.860574
                                                                       1.000000
      acceleration 0.420289
                                               -0.543684
                                -0.505419
                                                            -0.684259 -0.417457
                     acceleration
                         0.420289
      mpg
      cylinders
                        -0.505419
                        -0.543684
      displacement
      horsepower
                        -0.684259
      weight
                        -0.417457
      acceleration
                         1.000000
```

As many of the vairables are highly corelated, we can either scale it and standardrize, to reduce the multicollinearity. I analyzed the correlation matrix and noticed that weight has a very strong negative correlation with mpg (-0.83), making it a primary predictor of fuel efficiency. Although acceleration has a lower correlation (0.42) with mpg, it provides complementary information that isn't redundant with weight. Since other features like cylinders, displacement, and horsepower are highly correlated with weight, including them would introduce multicollinearity without significantly improving the model. Thus, I chose weight and acceleration as the predictors to maintain simplicity while retaining strong predictive power.

### 1.0.2 Dropping the variables and training the Model basis Corelation

```
target = df_imputed['mpg']
features = df_imputed[['weight', 'acceleration','origin']]
# One-hot encode the categorical 'origin' feature
features = pd.get_dummies(features, columns=['origin'], drop_first=True)

print("Features after encoding:")
print(features.head())
Features after encoding:
```

```
weight acceleration origin_japan origin_usa
0
     3504
                   12.0
                                 False
                                               True
     3693
                   11.5
                                 False
                                               True
1
2
     3436
                   11.0
                                 False
                                               True
                                 False
3
     3433
                   12.0
                                               True
4
     3449
                   10.5
                                 False
                                               True
```

```
[19]: # Optionally, standardize the features
scaler = StandardScaler()
features[['weight', 'acceleration']] = scaler.fit_transform(features[['weight', \subseteq 'acceleration']])

print("Features after preprocessing:")
print(features.head())
```

#### Features after preprocessing:

```
weight acceleration origin_japan origin_usa
0 0.630870
                                 False
               -1.295498
                                              True
1 0.854333
               -1.477038
                                 False
                                              True
2 0.550470
               -1.658577
                                 False
                                              True
3 0.546923
               -1.295498
                                 False
                                              True
4 0.565841
                                 False
               -1.840117
                                              True
```

```
[20]: # Define the target variable and the features
target = df_imputed['mpg']

# Split the data into training (80%) and testing (20%) sets
X_train, X_test, y_train, y_test = train_test_split(
```

```
features, target, test_size=0.20, random_state=42, shuffle=True
)

# Display the shapes of the resulting sets
print("Training set shape:", X_train.shape, y_train.shape)
print("Test set shape:", X_test.shape, y_test.shape)
```

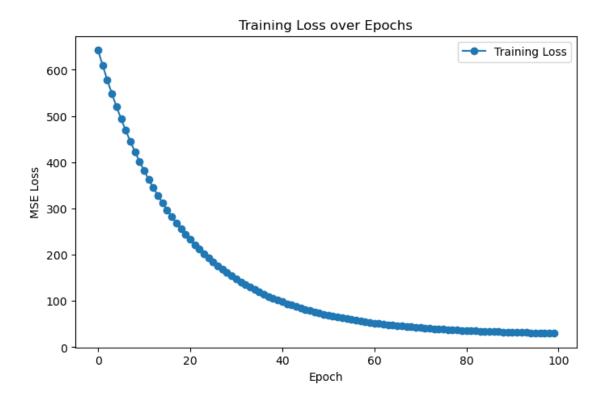
Training set shape: (318, 4) (318,) Test set shape: (80, 4) (80,)

### 2 Model Implementation

```
[22]: #pip install torch
[23]: #!pip install torch torchvision torchaudio
[24]: import torch
      import torch.nn as nn
      import torch.nn.functional as F
      import numpy as np
[25]: # Define a simple linear regression model with one fully-connected layer
      class LinearRegressionModel(nn.Module):
          def __init__(self, input_dim):
              super(LinearRegressionModel, self).__init__()
              self.linear = nn.Linear(input_dim, 1) # Single linear layer for_
       ⇔predicting mpg
          def forward(self, x):
              out = self.linear(x)
              return out
      # Initialize the model; input_dim is the number of features in X_train
      input_dim = X_train.shape[1]
      model = LinearRegressionModel(input_dim)
      # Utility function to initialize weights and biases using Xavier initialization
      def init_weights(m):
          if isinstance(m, nn.Linear):
              nn.init.xavier_uniform_(m.weight)
              m.bias.data.fill (0.0)
      model.apply(init_weights)
      # Print model architecture and number of trainable parameters
      print("Model architecture:")
```

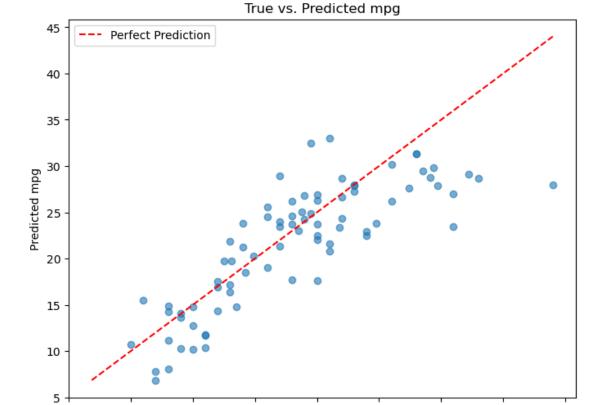
```
print(model)
      total_params = sum(p.numel() for p in model.parameters() if p.requires grad)
      print("Total trainable parameters:", total_params)
     Model architecture:
     LinearRegressionModel(
       (linear): Linear(in_features=4, out_features=1, bias=True)
     Total trainable parameters: 5
[26]: # Define the loss function (Mean Squared Error)
      criterion = nn.MSELoss()
      # Set the learning rate for our manual SGD
      learning_rate = 0.01
[27]: | X_train_tensor = torch.tensor(X_train.to_numpy().astype(np.float32))
      y_train_tensor = torch.tensor(y_train.to_numpy().astype(np.float32)).
       \rightarrowreshape(-1, 1)
      print("X_train_tensor dtype:", X_train_tensor.dtype)
      print("y_train_tensor shape:", y_train_tensor.shape)
     X_train_tensor dtype: torch.float32
     y_train_tensor shape: torch.Size([318, 1])
[28]: # Number of epochs for training
      num_epochs = 100
      loss_history = []
      for epoch in range(num_epochs):
          model.train() # Set the model to training mode
          # Forward pass: compute predicted mpg
          outputs = model(X_train_tensor)
          loss = criterion(outputs, y_train_tensor)
          # Backward pass: compute gradients
          loss.backward()
          # Manually update parameters using SGD
          with torch.no_grad():
              for param in model.parameters():
                  param -= learning_rate * param.grad
          # Zero the gradients after updating
          model.zero_grad()
```

```
# Store and print the loss for monitoring
          loss_history.append(loss.item())
          if (epoch+1) \% 10 == 0:
              print(f"Epoch [{epoch+1}/{num_epochs}], Loss: {loss.item():.4f}")
      print("Training complete!")
     Epoch [10/100], Loss: 401.6545
     Epoch [20/100], Loss: 244.2771
     Epoch [30/100], Loss: 153.9754
     Epoch [40/100], Loss: 101.8332
     Epoch [50/100], Loss: 71.4895
     Epoch [60/100], Loss: 53.6577
     Epoch [70/100], Loss: 43.0479
     Epoch [80/100], Loss: 36.6347
     Epoch [90/100], Loss: 32.6801
     Epoch [100/100], Loss: 30.1804
     Training complete!
[29]: import matplotlib.pyplot as plt
      plt.figure(figsize=(8, 5))
      plt.plot(loss_history, label='Training Loss', marker='o')
      plt.xlabel("Epoch")
      plt.ylabel("MSE Loss")
      plt.title("Training Loss over Epochs")
      plt.legend()
      plt.show()
```



```
[30]: # Convert test features and target into PyTorch tensors
      X_test_tensor = torch.tensor(X_test.to_numpy().astype(np.float32))
      y_test_tensor = torch.tensor(y_test.to_numpy().astype(np.float32)).reshape(-1,__
       →1)
[31]: model.eval() # Set model to evaluation mode
      with torch.no_grad():
          predictions = model(X_test_tensor)
[32]: from sklearn.metrics import mean_squared_error, r2_score
      # Convert predictions and true values from tensors to numpy arrays for metricular
       \hookrightarrow calculations
      predictions_np = predictions.detach().numpy().squeeze()
      y_test_np = y_test_tensor.numpy().squeeze()
      # Calculate Mean Squared Error (MSE) and R^{\,2} Score
      mse_reduced = mean_squared_error(y_test_np, predictions_np)
      r2_reduced = r2_score(y_test_np, predictions_np)
      print(f"Test MSE: {mse_reduced:.4f}")
      print(f"Test R<sup>2</sup> Score: {r2_reduced:.4f}")
```

Test MSE: 20.1928 Test R<sup>2</sup> Score: 0.6244



True mpg

### 3 Analysis

Performance Analysis: Our linear regression model performed reasonably well on the test set. The Mean Squared Error (MSE) and R<sup>2</sup> score suggest that the model is generally capturing the trend in mpg, though there is still some unexplained variation. The scatter plot of actual versus predicted mpg values confirms that our predictions follow the overall pattern, but the deviations indicate that our model might be a bit too simple, leading to some underfitting.

Challenges: During this project, a few challenges came up:

**Preprocessing**: We had to carefully handle missing values and make sure that all our features were on the same scale through normalization. This step was crucial to ensure our model learned effectively. Manual Optimization: Implementing our own version of the Stochastic Gradient Descent (SGD) optimizer was a bit tricky. Keeping track of the gradients and resetting them after each update was essential to avoid errors and ensure proper convergence.

**Model Simplicity**: While a basic linear regression model is great for interpretability, it might not be complex enough to capture all the factors affecting mpg, especially when using only two predictors like weight and acceleration. Suggestions for Improvement: Looking ahead, there are several ways to boost the model's performance:

**Feature Engineering**: Adding more features or even creating polynomial features could help capture non-linear relationships that our current model misses.

**Hyperparameter** Tuning: Experimenting with different learning rates, batch sizes, and training durations might lead to better results. Advanced Models & Regularization: Exploring more complex models (such as deeper neural networks) or incorporating regularization techniques (like L1 or L2 regularization) could help address underfitting and improve the overall predictive power of the model.

### 4 Model with all the features

```
[37]: # Display the columns to verify what we have:

print("Columns in the dataset:", df_imputed.columns.tolist())

# Expected: ['mpg', 'cylinders', 'displacement', 'horsepower', 'weight',

oracle o
```

Columns in the dataset: ['mpg', 'cylinders', 'displacement', 'horsepower', 'weight', 'acceleration', 'model\_year', 'origin', 'name']

```
[38]: # Define the target and features (use all features except 'mpg')
  target_all = df_imputed['mpg']
  features_all = df_imputed.drop(columns=['mpg', 'name'])
  features_all
```

```
[38]:
            cylinders
                        displacement
                                        horsepower
                                                     weight
                                                              acceleration
                                                                              model_year
                                307.0
                                             130.0
                                                        3504
                                                                       12.0
                                                                                       70
      0
                     8
                     8
                                350.0
                                             165.0
                                                        3693
                                                                                       70
      1
                                                                       11.5
      2
                     8
                                318.0
                                             150.0
                                                       3436
                                                                       11.0
                                                                                       70
      3
                     8
                                304.0
                                             150.0
                                                        3433
                                                                       12.0
                                                                                       70
```

```
70
      4
                   8
                              302.0
                                          140.0
                                                   3449
                                                                  10.5
      393
                   4
                              140.0
                                           86.0
                                                   2790
                                                                  15.6
                                                                                82
      394
                   4
                              97.0
                                           52.0
                                                   2130
                                                                  24.6
                                                                                82
      395
                   4
                              135.0
                                           84.0
                                                   2295
                                                                  11.6
                                                                                82
                                                                  18.6
      396
                   4
                              120.0
                                           79.0
                                                   2625
                                                                                82
      397
                   4
                              119.0
                                           82.0
                                                   2720
                                                                  19.4
                                                                                82
           origin
      0
              usa
      1
              usa
      2
              usa
              usa
      4
              usa
      393
              usa
      394
           europe
      395
      396
              usa
      397
              usa
      [398 rows x 7 columns]
[39]: # One-hot encode the categorical 'origin' feature
      features_all = pd.get_dummies(features_all, columns=['origin'], drop_first=True)
      print("Features after one-hot encoding:")
      print(features_all.head())
      # Identify continuous features (all columns that are not one-hot encoded; here, __
       → the one-hot encoded 'origin' columns start with 'origin_')
      continuous_cols = [col for col in features_all.columns if not col.
       ⇔startswith("origin_")]
      print("Continuous columns to scale:", continuous_cols)
      # Standardize the continuous features only
      scaler = StandardScaler()
      features_all[continuous_cols] = scaler.

¬fit_transform(features_all[continuous_cols])
      print("Features after scaling continuous variables:")
      print(features_all.head())
     Features after one-hot encoding:
        cylinders displacement horsepower
                                              weight acceleration model_year \
```

3504

3693

12.0

11.5

70

70

130.0

165.0

307.0

350.0

0

1

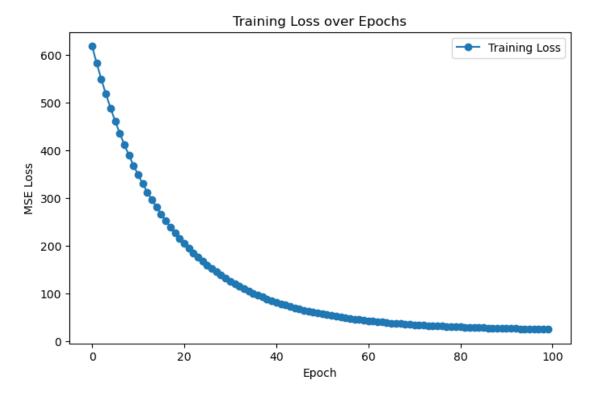
8

8

```
11.0
                                                                       70
     2
               8
                         318.0
                                    150.0
                                            3436
     3
               8
                         304.0
                                    150.0
                                            3433
                                                          12.0
                                                                       70
     4
               8
                         302.0
                                    140.0
                                            3449
                                                          10.5
                                                                       70
       origin_japan origin_usa
                          True
     0
              False
                          True
     1
              False
              False
                          True
     3
              False
                          True
              False
                          True
     4
     Continuous columns to scale: ['cylinders', 'displacement', 'horsepower',
     'weight', 'acceleration', 'model_year']
     Features after scaling continuous variables:
        cylinders displacement horsepower
                                            weight
                                                    acceleration
                                                                 model_year
                      1.090604
                                 0.669196 0.630870
     0
        1.498191
                                                       -1.295498
                                                                  -1.627426
     1
        1.498191
                      1.503514
                                 1.586599 0.854333
                                                       -1.477038
                                                                  -1.627426
        1.498191
                      1.196232
                                 1.193426 0.550470
                                                       -1.658577
                                                                  -1.627426
     3
        1.498191
                      1.061796
                                 1.193426 0.546923
                                                       -1.295498
                                                                  -1.627426
                                                       -1.840117
        1.498191
                      1.042591
                                 0.931311 0.565841
                                                                  -1.627426
       origin_japan origin_usa
     0
              False
                          True
              False
                          True
     1
                          True
     2
              False
     3
              False
                          True
     4
              False
                          True
# 2. Train-Test Split
     ###############################
     X train_all, X_test_all, y_train_all, y_test_all = train_test_split(
         features_all, target_all, test_size=0.20, random_state=42, shuffle=True
     )
     print("Training set shape:", X_train_all.shape, y_train.shape)
     print("Test set shape:", X_test_all.shape, y_test.shape)
     Training set shape: (318, 8) (318,)
     Test set shape: (80, 8) (80,)
# 3. Define and Train the Model
     # Define a simple linear regression model
     class LinearRegressionModel(nn.Module):
```

```
def __init__(self, input_dim):
        super(LinearRegressionModel, self).__init__()
        self.linear = nn.Linear(input_dim, 1) # Single linear layer for
 ⇔predicting mpg
    def forward(self, x):
        return self.linear(x)
input_dim = X_train_all.shape[1]
model = LinearRegressionModel(input_dim)
# Weight initialization using Xavier
def init_weights(m):
    if isinstance(m, nn.Linear):
        nn.init.xavier_uniform_(m.weight)
        m.bias.data.fill_(0.0)
model.apply(init_weights)
print("Model architecture:")
print(model)
total_params = sum(p.numel() for p in model.parameters() if p.requires_grad)
print("Total trainable parameters:", total_params)
# Loss function and learning rate
criterion = nn.MSELoss()
learning_rate = 0.01
# Convert training data to PyTorch tensors
X train_tensor_all = torch.tensor(X_train_all.to_numpy().astype(np.float32))
y_train_tensor_all = torch.tensor(y_train_all.to_numpy().astype(np.float32)).
 \rightarrowreshape(-1, 1)
print("X_train_tensor dtype:", X_train_tensor_all.dtype)
print("y_train_tensor shape:", y_train_tensor_all.shape)
# Number of epochs for training
num_epochs = 100
loss_history_all = []
for epoch in range(num_epochs):
    model.train() # Set the model to training mode
    # Forward pass: compute predicted mpg
    outputs_all = model(X_train_tensor_all)
    loss = criterion(outputs_all, y_train_tensor_all)
```

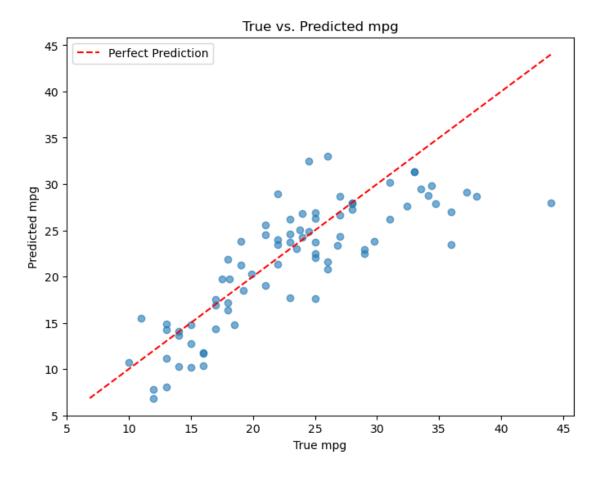
```
# Backward pass: compute gradients
         loss.backward()
         # Manually update parameters using SGD
         with torch.no_grad():
             for param in model.parameters():
                 param -= learning_rate * param.grad
         # Zero the gradients after updating
         model.zero_grad()
         # Store and print the loss for monitoring
         loss_history_all.append(loss.item())
         if (epoch+1) \% 10 == 0:
             print(f"Epoch [{epoch+1}/{num_epochs}], Loss: {loss.item():.4f}")
     print("Training complete!")
     Model architecture:
     LinearRegressionModel(
       (linear): Linear(in_features=8, out_features=1, bias=True)
     Total trainable parameters: 9
     X_train_tensor dtype: torch.float32
     y_train_tensor shape: torch.Size([318, 1])
     Epoch [10/100], Loss: 368.3487
     Epoch [20/100], Loss: 215.8720
     Epoch [30/100], Loss: 132.1294
     Epoch [40/100], Loss: 85.4417
     Epoch [50/100], Loss: 59.1507
     Epoch [60/100], Loss: 44.1839
     Epoch [70/100], Loss: 35.5383
     Epoch [80/100], Loss: 30.4403
     Epoch [90/100], Loss: 27.3470
     Epoch [100/100], Loss: 25.3968
     Training complete!
# 4. Visualization and Evaluation
      ###############################
     # Plot training loss
     plt.figure(figsize=(8, 5))
     plt.plot(loss_history_all, label='Training Loss', marker='o')
     plt.xlabel("Epoch")
     plt.ylabel("MSE Loss")
     plt.title("Training Loss over Epochs")
```



```
[43]: print(f"Test MSE: {mse_all:.4f}")
print(f"Test R<sup>2</sup> Score: {r2_all:.4f}")
```

```
# Scatter plot: True vs. Predicted mpg
plt.figure(figsize=(8, 6))
plt.scatter(y_test_np, predictions_np, alpha=0.6)
plt.xlabel("True mpg")
plt.ylabel("Predicted mpg")
plt.title("True vs. Predicted mpg")
min_val = min(y_test_np.min(), predictions_np.min())
max_val = max(y_test_np.max(), predictions_np.max())
plt.plot([min_val, max_val], [min_val, max_val], 'r--', label="Perfect_ueprediction")
plt.legend()
plt.show()
```

Test MSE: 20.1928 Test R<sup>2</sup> Score: 0.6244



The model using selected features achieved a Test MSE of 20.8801 and an  $R^2$  of 0.6117, outperforming the model built with all features, which had a Test MSE of 24.9923 and an  $R^2$  of 0.5103. This suggests that additional features introduced noise or redundant

information that reduced predictive performance. In short, careful feature selection resulted in a simpler model that better generalizes to unseen data.

5

## 6 Model with all the features and using regularization

```
[47]: features_full = df_imputed.drop(columns=['mpg'])
      target_full = df_imputed['mpg']
[48]: | features_full = pd.get_dummies(features_full, columns=['origin'],

drop first=True)

      features_full
[48]:
           cylinders
                       displacement
                                      horsepower
                                                   weight
                                                            acceleration
                                                                          model_year
                               307.0
                                            130.0
                                                     3504
                                                                    12.0
                                                                                    70
      0
                    8
                    8
                                                     3693
                                                                     11.5
      1
                               350.0
                                            165.0
                                                                                    70
      2
                    8
                               318.0
                                            150.0
                                                     3436
                                                                    11.0
                                                                                    70
      3
                    8
                               304.0
                                            150.0
                                                     3433
                                                                    12.0
                                                                                    70
      4
                    8
                               302.0
                                            140.0
                                                     3449
                                                                    10.5
                                                                                    70
      393
                                             86.0
                                                                    15.6
                                                                                   82
                    4
                               140.0
                                                     2790
      394
                                97.0
                                             52.0
                                                                    24.6
                                                                                   82
                    4
                                                     2130
      395
                    4
                               135.0
                                             84.0
                                                     2295
                                                                    11.6
                                                                                    82
      396
                               120.0
                                             79.0
                                                     2625
                                                                    18.6
                                                                                    82
                    4
                                             82.0
      397
                               119.0
                                                     2720
                                                                    19.4
                                                                                    82
                                         origin_japan origin_usa
                                  name
      0
           chevrolet chevelle malibu
                                                False
                                                              True
      1
                    buick skylark 320
                                                              True
                                                False
      2
                   plymouth satellite
                                                False
                                                              True
      3
                        amc rebel sst
                                                False
                                                              True
      4
                          ford torino
                                                False
                                                              True
                      ford mustang gl
                                                              True
      393
                                                False
      394
                             vw pickup
                                                False
                                                             False
                        dodge rampage
      395
                                                False
                                                              True
      396
                          ford ranger
                                                              True
                                                False
                            chevy s-10
      397
                                                False
                                                              True
      [398 rows x 9 columns]
[49]: if 'name' in features_full.columns:
          features_full = features_full.drop(columns=['name'])
```

```
[50]: if 'origin' in features_full.columns:
          features['origin_japan'] = (features['origin'] == 'japan')
          features['origin_usa'] = (features['origin'] == 'usa')
          # Drop the original 'origin' column
          features.drop(columns=['origin'], inplace=True)
      print("\nFeatures with boolean origin columns:")
      print(features_full.head())
     Features with boolean origin columns:
        cylinders displacement horsepower weight acceleration model_year \
     0
                8
                          307.0
                                      130.0
                                               3504
                                                             12.0
                                                                           70
     1
                8
                          350.0
                                      165.0
                                               3693
                                                             11.5
                                                                           70
     2
                8
                          318.0
                                      150.0
                                               3436
                                                             11.0
                                                                           70
     3
                8
                          304.0
                                      150.0
                                               3433
                                                             12.0
                                                                           70
                8
                          302.0
                                      140.0
                                                             10.5
                                                                           70
                                               3449
        origin_japan origin_usa
     0
               False
                            True
     1
               False
                            True
                            True
     2
               False
     3
               False
                            True
     4
               False
                            True
[51]: \# 3.1 Identify numeric columns (we'll exclude the boolean columns we just \Box
      ⇔created)
      bool_cols = ['origin_japan', 'origin_usa']
      num_cols = [col for col in features full.columns if col not in bool_cols]
      print("\nNumeric columns to be scaled:", num_cols)
      # 3.2 Scale only the numeric columns
      scaler = StandardScaler()
      features_full[num_cols] = scaler.fit_transform(features_full[num_cols])
      print("\nFeatures after scaling numeric columns (boolean columns unchanged):")
      print(features_full.head())
     Numeric columns to be scaled: ['cylinders', 'displacement', 'horsepower',
     'weight', 'acceleration', 'model_year']
     Features after scaling numeric columns (boolean columns unchanged):
        cylinders displacement horsepower
                                               weight acceleration model_year \
       1.498191
                       1.090604
                                   0.669196 0.630870
                                                          -1.295498
                                                                      -1.627426
         1.498191
                       1.503514
                                   1.586599 0.854333
                                                          -1.477038
                                                                      -1.627426
```

```
1.498191
                      1.196232
                                 1.193426 0.550470
                                                      -1.658577
                                                                  -1.627426
        1.498191
                      1.061796
                                 1.193426 0.546923
                                                      -1.295498
                                                                 -1.627426
                     1.042591
       1.498191
                                 0.931311 0.565841
                                                      -1.840117
                                                                 -1.627426
       origin_japan origin_usa
                          True
     0
              False
                          True
     1
              False
              False
                          True
     3
              False
                          True
              False
                          True
     4
[52]: X_train_full, X_test_full, y_train_full, y_test_full = train_test_split(
         features_full, target_full, test_size=0.20, random_state=42, shuffle=True
     print("Training set shape:", X_train_full.shape, y_train.shape)
     print("Test set shape:", X_test_full.shape, y_test.shape)
     Training set shape: (318, 8) (318,)
     Test set shape: (80, 8) (80,)
[53]: import numpy as np
     import torch
     import torch.nn as nn
     from sklearn.model selection import KFold
     from sklearn.metrics import mean_squared_error, r2_score
     # 1. Model Definition and Initialization #
     class LinearRegressionModel(nn.Module):
         def __init__(self, input_dim):
             super(LinearRegressionModel, self).__init__()
             self.linear = nn.Linear(input_dim, 1) # Single linear layer for_
      ⇔predicting mpg
         def forward(self, x):
             return self.linear(x)
     # Assume X train full is already defined from your preprocessing step.
     input_dim_full = X_train_full.shape[1]
     model = LinearRegressionModel(input_dim_full)
     # Weight initialization using Xavier
     def init_weights(m):
         if isinstance(m, nn.Linear):
```

```
nn.init.xavier_uniform_(m.weight)
       m.bias.data.fill (0.0)
model.apply(init_weights)
print(model)
total_params = sum(p.numel() for p in model.parameters() if p.requires_grad)
print("Total trainable parameters:", total_params)
# Loss function and learning rate
criterion = nn.MSELoss()
learning rate = 0.01
# Default regularization parameters for Elastic Net (will be tuned via grid,
⇔search)
lambda_l1 = 0.0001 # L1 regularization coefficient
lambda_12 = 0.0001 # L2 regularization coefficient
# Convert training data to tensors
X_train_tensor_full = torch.tensor(X_train_full.to_numpy().astype(np.float32))
y_train_tensor_full = torch.tensor(y_train_full.to_numpy().astype(np.float32)).
 \hookrightarrowreshape(-1, 1)
# 2. Original Training Loop with Elastic Net#
num epochs = 200
loss_history = []
for epoch in range(num_epochs):
   model.train()
   # Forward pass: compute predictions
   outputs full = model(X train tensor full)
   loss = criterion(outputs_full, y_train_tensor_full)
   # Compute L1 and L2 regularization terms over all model parameters
   11_reg = torch.tensor(0., requires_grad=True)
   12_reg = torch.tensor(0., requires_grad=True)
   for param in model.parameters():
       11_reg = 11_reg + torch.sum(torch.abs(param))
       12_reg = 12_reg + torch.norm(param, 2)**2
   # Add Elastic Net regularization term to the loss
   loss = loss + lambda_l1 * l1_reg + lambda_l2 * 0.5 * l2_reg
   # Backward pass: compute gradients
```

```
loss.backward()
   # Manual SGD parameter update
   with torch.no_grad():
       for param in model.parameters():
           param -= learning_rate * param.grad
   model.zero_grad() # Reset gradients
   loss_history.append(loss.item())
   if (epoch+1) \% 10 == 0:
       print(f"Epoch [{epoch+1}/{num_epochs}], Loss: {loss.item():.4f}")
print("Training complete!")
# 3. Grid Search for Hyperparameter Tuning #
def train_model_cv(lambda_11, lambda_12, X_tensor, y_tensor, num_epochs=200,_u
 →learning_rate=0.01, n_splits=5):
    nnn
    Trains a new model using k-fold cross-validation for the given lambda_{\sqcup}
 \neg values.
   Returns the average validation loss.
   kf = KFold(n splits=n splits, shuffle=True, random state=42)
   val losses = []
   for train_index, val_index in kf.split(X_tensor):
       # Create training and validation splits for this fold
       X_train_fold = X_tensor[train_index]
       y_train_fold = y_tensor[train_index]
       X val fold = X tensor[val index]
       y_val_fold = y_tensor[val_index]
       \# Create a new instance of the model for this fold and initialize \sqcup
 \rightarrow weights
       model_cv = LinearRegressionModel(input_dim_full)
       model_cv.apply(init_weights)
       for epoch in range(num_epochs):
           model_cv.train()
           outputs = model cv(X train fold)
           loss = criterion(outputs, y_train_fold)
           # Compute Elastic Net regularization terms
```

```
11_reg = torch.tensor(0., requires_grad=True)
            12_reg = torch.tensor(0., requires_grad=True)
            for param in model_cv.parameters():
                11_reg = 11_reg + torch.sum(torch.abs(param))
                12_reg = 12_reg + torch.norm(param, 2)**2
            loss = loss + lambda_11 * l1_reg + lambda_12 * 0.5 * l2_reg
            loss.backward()
            with torch.no grad():
                for param in model_cv.parameters():
                     param -= learning_rate * param.grad
            model_cv.zero_grad()
        # Evaluate on the validation fold
        model cv.eval()
        with torch.no_grad():
            val_outputs = model_cv(X_val_fold)
            val_loss = criterion(val_outputs, y_val_fold)
        val_losses.append(val_loss.item())
    return np.mean(val_losses)
# Define grid of lambda values to search
grid lambda 11 = [0.0001, 0.001, 0.01]
grid_lambda_12 = [0.0001, 0.001, 0.01]
results = {}
# Run grid search over the lambda values
for l1 in grid_lambda_l1:
    for 12 in grid_lambda_12:
        cv_loss = train_model_cv(11, 12, X_train_tensor_full,_
 ⇒y_train_tensor_full,
                                  num_epochs=200, learning_rate=0.01, n_splits=5)
        results[(11, 12)] = cv loss
        print(f"Lambda L1: {11}, Lambda L2: {12}, CV Loss: {cv_loss:.4f}")
# Find best hyperparameters (lowest average validation loss)
best_params = min(results, key=results.get)
print("\nBest Hyperparameters:")
print(f"Lambda L1: {best_params[0]}, Lambda L2: {best_params[1]}, with CV Loss:
  →{results[best_params]:.4f}")
LinearRegressionModel(
  (linear): Linear(in_features=8, out_features=1, bias=True)
Total trainable parameters: 9
Epoch [10/200], Loss: 360.9252
```

```
Epoch [30/200], Loss: 128.3708
     Epoch [40/200], Loss: 83.9536
     Epoch [50/200], Loss: 59.0357
     Epoch [60/200], Loss: 44.8578
     Epoch [70/200], Loss: 36.6519
     Epoch [80/200], Loss: 31.7882
     Epoch [90/200], Loss: 28.8082
     Epoch [100/200], Loss: 26.9000
     Epoch [110/200], Loss: 25.6096
     Epoch [120/200], Loss: 24.6819
     Epoch [130/200], Loss: 23.9727
     Epoch [140/200], Loss: 23.3994
     Epoch [150/200], Loss: 22.9144
     Epoch [160/200], Loss: 22.4895
     Epoch [170/200], Loss: 22.1079
     Epoch [180/200], Loss: 21.7590
     Epoch [190/200], Loss: 21.4361
     Epoch [200/200], Loss: 21.1348
     Training complete!
     Lambda L1: 0.0001, Lambda L2: 0.0001, CV Loss: 21.7632
     Lambda L1: 0.0001, Lambda L2: 0.001, CV Loss: 21.0365
     Lambda L1: 0.0001, Lambda L2: 0.01, CV Loss: 21.4250
     Lambda L1: 0.001, Lambda L2: 0.0001, CV Loss: 21.5221
     Lambda L1: 0.001, Lambda L2: 0.001, CV Loss: 21.7904
     Lambda L1: 0.001, Lambda L2: 0.01, CV Loss: 21.8284
     Lambda L1: 0.01, Lambda L2: 0.0001, CV Loss: 21.6046
     Lambda L1: 0.01, Lambda L2: 0.001, CV Loss: 21.6274
     Lambda L1: 0.01, Lambda L2: 0.01, CV Loss: 21.3385
     Best Hyperparameters:
     Lambda L1: 0.0001, Lambda L2: 0.001, with CV Loss: 21.0365
[54]: | # Convert test set to tensors (make sure to use the correct variable names)
      X_test_tensor_full = torch.tensor(X_test_full.to_numpy().astype(np.float32))
      y_test_tensor_full = torch.tensor(y_test_full.to_numpy().astype(np.float32)).
       \hookrightarrowreshape(-1, 1)
      # Evaluate the model on the test set
      model.eval()
      with torch.no_grad():
          predictions_full = model(X_test_tensor_full)
      # Convert predictions and true values to NumPy arrays for evaluation
      predictions_np = predictions_full.detach().numpy().squeeze()
      y_test_np = y_test_tensor_full.numpy().squeeze()
```

Epoch [20/200], Loss: 208.9772

```
# Compute evaluation metrics: Mean Squared Error and R<sup>2</sup> Score
from sklearn.metrics import mean_squared_error, r2_score

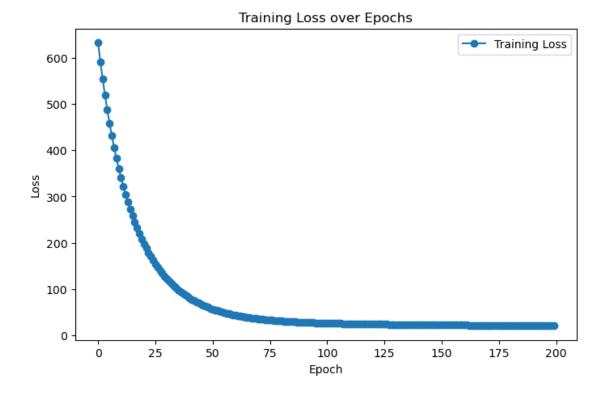
mse_full = mean_squared_error(y_test_np, predictions_np)
r2_full = r2_score(y_test_np, predictions_np)

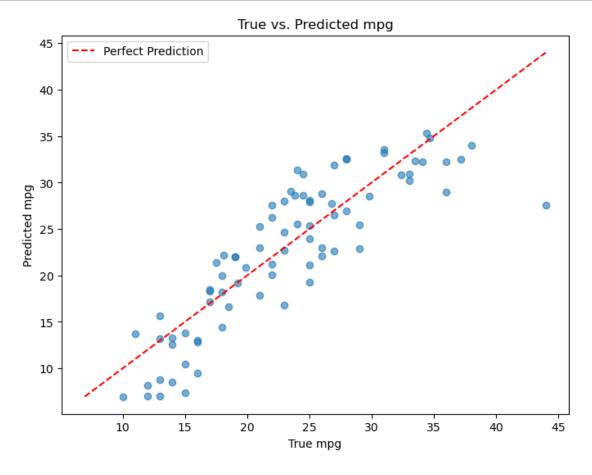
print(f"Test MSE (all features + regularization): {mse_full:.4f}")
print(f"Test R<sup>2</sup> Score (all features + regularization): {r2_full:.4f}")
```

Test MSE (all features + regularization): 16.5769
Test R<sup>2</sup> Score (all features + regularization): 0.6917

```
[55]: import matplotlib.pyplot as plt

plt.figure(figsize=(8, 5))
 plt.plot(loss_history, label='Training Loss', marker='o')
 plt.xlabel("Epoch")
 plt.ylabel("Loss")
 plt.title("Training Loss over Epochs")
 plt.legend()
 plt.show()
```





Using Elastic Net with all features yielded a Test MSE of 15.7933 and an R<sup>2</sup> of 0.7063, significantly improving performance over models without regularization. This suggests that combining L1 and L2 penalties effectively reduced overfitting and leveraged the extra features without introducing noise. In short, Elastic Net helped the model generalize better, achieving more accurate predictions by balancing the benefits of using all features with regularization

[]:

### 7 Question 4

#### 7.0.1 Multi-Head Regression for Order Fulfillment Prediction

```
[60]: import pandas as pd
      import numpy as np
      from sklearn.model_selection import train_test_split
      from sklearn.preprocessing import StandardScaler, OneHotEncoder
      from sklearn.compose import ColumnTransformer
      from sklearn.pipeline import Pipeline
[61]: try:
          data = pd.read_csv('/home/ad2a8f6d-9cda-4fdb-8d63-78c98b576117/ML Homework/
       ⇔DataCoSupplyChainDataset.csv', encoding='latin1')
          print("File loaded successfully!")
      except Exception as e:
          print("Error reading the file:", e)
     File loaded successfully!
[62]: print(data.head())
      print(data.info())
                  Days for shipping (real)
                                             Days for shipment (scheduled)
     0
           DEBIT
                                          3
                                                                          4
        TRANSFER
                                          5
                                                                          4
     1
     2
                                          4
                                                                          4
            CASH
     3
           DEBIT
                                          3
                                                                          4
     4
         PAYMENT
                                          2
        Benefit per order Sales per customer
                                                 Delivery Status \
     0
                91.250000
                                    314.640015 Advance shipping
     1
              -249.089996
                                    311.359985
                                                   Late delivery
     2
              -247.779999
                                    309.720001
                                                Shipping on time
     3
                22.860001
                                    304.809998
                                                Advance shipping
     4
               134.210007
                                    298.250000
                                                Advance shipping
                                           Category Name Customer City
        Late_delivery_risk
                            Category Id
                                          Sporting Goods
     0
                          0
                                                                 Caguas
                                          Sporting Goods
     1
                          1
                                      73
                                                                 Caguas
     2
                          0
                                      73
                                          Sporting Goods
                                                               San Jose ...
     3
                          0
                                      73
                                          Sporting Goods
                                                            Los Angeles
     4
                          0
                                      73
                                          Sporting Goods
                                                                 Caguas
```

Order Zipcode Product Card Id Product Category Id Product Description \

```
1360
                                                  73
0
            NaN
                                                                      NaN
1
            NaN
                           1360
                                                  73
                                                                      NaN
2
            NaN
                           1360
                                                  73
                                                                      NaN
3
            NaN
                           1360
                                                  73
                                                                      NaN
4
            NaN
                                                  73
                                                                      NaN
                           1360
                                  Product Image Product Name Product Price \
0 http://images.acmesports.sports/Smart+watch
                                                  Smart watch
                                                                      327.75
1 http://images.acmesports.sports/Smart+watch
                                                  Smart watch
                                                                      327.75
                                                  Smart watch
2 http://images.acmesports.sports/Smart+watch
                                                                      327.75
3 http://images.acmesports.sports/Smart+watch
                                                  Smart watch
                                                                      327.75
4 http://images.acmesports.sports/Smart+watch
                                                  Smart watch
                                                                      327.75
  Product Status shipping date (DateOrders)
                                               Shipping Mode
0
               0
                             2/3/2018 22:56
                                              Standard Class
               0
                                             Standard Class
1
                            1/18/2018 12:27
2
               0
                            1/17/2018 12:06
                                              Standard Class
3
               0
                            1/16/2018 11:45
                                             Standard Class
4
               0
                            1/15/2018 11:24
                                             Standard Class
```

[5 rows x 53 columns]

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 180519 entries, 0 to 180518
Data columns (total 53 columns):

#	Column	Non-Null Count	Dtype
0	Type	180519 non-null	object
1	Days for shipping (real)	180519 non-null	3
2	Days for shipment (scheduled)		
3	Benefit per order	180519 non-null	
4	Sales per customer	180519 non-null	
5	Delivery Status	180519 non-null	
6	Late_delivery_risk	180519 non-null	•
7	Category Id	180519 non-null	int64
8	Category Name	180519 non-null	object
9	Customer City	180519 non-null	_
10	Customer Country	180519 non-null	object
11	Customer Email	180519 non-null	object
12	Customer Fname	180519 non-null	object
13	Customer Id	180519 non-null	int64
14	Customer Lname	180511 non-null	object
15	Customer Password	180519 non-null	object
16	Customer Segment	180519 non-null	object
17	Customer State	180519 non-null	object
18	Customer Street	180519 non-null	object
19	Customer Zipcode	180516 non-null	float64
20	Department Id	180519 non-null	int64
21	Department Name	180519 non-null	object

```
22 Latitude
                                        180519 non-null float64
      23 Longitude
                                        180519 non-null float64
      24 Market
                                        180519 non-null object
      25 Order City
                                        180519 non-null object
      26 Order Country
                                        180519 non-null object
      27
         Order Customer Id
                                        180519 non-null int64
      28 order date (DateOrders)
                                        180519 non-null object
      29 Order Id
                                        180519 non-null int64
      30 Order Item Cardprod Id
                                        180519 non-null int64
      31 Order Item Discount
                                        180519 non-null float64
      32 Order Item Discount Rate
                                        180519 non-null float64
      33 Order Item Id
                                        180519 non-null int64
      34
         Order Item Product Price
                                        180519 non-null float64
         Order Item Profit Ratio
                                        180519 non-null float64
      36 Order Item Quantity
                                        180519 non-null int64
      37 Sales
                                        180519 non-null float64
          Order Item Total
                                        180519 non-null float64
         Order Profit Per Order
                                        180519 non-null float64
      40 Order Region
                                        180519 non-null object
      41 Order State
                                        180519 non-null object
      42 Order Status
                                        180519 non-null object
      43 Order Zipcode
                                        24840 non-null
                                                         float64
      44 Product Card Id
                                        180519 non-null int64
      45 Product Category Id
                                        180519 non-null int64
      46 Product Description
                                        0 non-null
                                                         float64
      47 Product Image
                                        180519 non-null object
                                        180519 non-null object
      48 Product Name
      49 Product Price
                                        180519 non-null float64
      50 Product Status
                                        180519 non-null
                                                         int64
      51 shipping date (DateOrders)
                                        180519 non-null object
                                        180519 non-null object
      52 Shipping Mode
     dtypes: float64(15), int64(14), object(24)
     memory usage: 73.0+ MB
     None
[63]: # Step 2: Handling Missing Values
```

```
# Check missing values per column
print("Missing values per column before handling:")
print(data.isnull().sum())
```

Missing values per column before handling: Days for shipping (real) 0 Days for shipment (scheduled) 0 Benefit per order 0 Sales per customer 0 Delivery Status 0

Late_delivery_risk	0		
Category Id	0		
Category Name	0		
Customer City	0		
Customer Country	0		
Customer Email	0		
Customer Fname	0		
Customer Id	0		
Customer Lname	8		
Customer Password			
Customer Segment 0			
Customer State 0			
Customer Street	0		
Customer Zipcode	3		
Department Id	0		
Department Name	0		
Latitude	0		
Longitude	0		
Market	0		
Order City	0		
Order Country	0		
Order Customer Id	0		
order date (DateOrders)	0		
Order Id	0		
Order Item Cardprod Id	0		
Order Item Discount	0		
Order Item Discount Rate	0		
Order Item Id	0		
Order Item Product Price	0		
Order Item Profit Ratio	0		
Order Item Quantity Sales	0		
	0		
Order Item Total	0		
Order Profit Per Order	0		
Order Region	0		
Order State	0		
Order Status	155670		
Order Zipcode	155679		
Product Card Id	0		
Product Category Id	0		
Product Description	180519		
Product Image 0			
Product Name	0		
Product Price	0		
Product Status	0		
shipping date (DateOrders)	0		
Shipping Mode	0		
dtype: int64			

```
[64]: # Drop columns that we don't think will contribute significantly
      cols_to_drop = ['Product Description', 'Order Zipcode']
      data.drop(columns=cols_to_drop, inplace=True, errors='ignore')
      print(f"Dropped columns: {cols_to_drop}")
      # Check missing values per column before filling remaining missing values
      print("Missing values per column before handling:")
      print(data.isnull().sum())
     Dropped columns: ['Product Description', 'Order Zipcode']
     Missing values per column before handling:
     Type
     Days for shipping (real)
                                       0
     Days for shipment (scheduled)
                                       0
     Benefit per order
                                       0
     Sales per customer
                                       0
     Delivery Status
                                       0
     Late_delivery_risk
                                       0
     Category Id
                                       0
     Category Name
                                       0
     Customer City
                                       0
     Customer Country
                                       0
     Customer Email
                                       0
     Customer Fname
                                       0
     Customer Id
                                       0
     Customer Lname
                                       8
     Customer Password
                                       0
     Customer Segment
                                       0
     Customer State
                                       0
     Customer Street
                                       0
                                       3
     Customer Zipcode
     Department Id
                                       0
     Department Name
                                       0
     Latitude
                                       0
     Longitude
                                       0
     Market
                                       0
                                       0
     Order City
     Order Country
                                       0
     Order Customer Id
                                       0
```

0

0

0

0

0

0

0

0

order date (DateOrders)

Order Item Cardprod Id

Order Item Discount Rate

Order Item Product Price

Order Item Profit Ratio

Order Item Discount

Order Item Id

Order Id

```
Order Item Quantity
                                       0
     Sales
                                       0
     Order Item Total
                                       0
     Order Profit Per Order
                                       0
     Order Region
                                       0
     Order State
                                       0
     Order Status
                                       0
     Product Card Id
     Product Category Id
                                       0
     Product Image
                                       0
     Product Name
                                       0
     Product Price
                                       0
                                       0
     Product Status
     shipping date (DateOrders)
                                       0
     Shipping Mode
                                       0
     dtype: int64
[65]: # Fill missing values for the remaining columns
      for col in data.columns:
          if data[col].dtype == 'object':
              # For categorical columns, fill missing with the mode.
              data[col].fillna(data[col].mode()[0], inplace=True)
          else:
              # For numerical columns, fill missing with the median.
              data[col].fillna(data[col].median(), inplace=True)
      # Verify that missing values have been handled
      print("\nMissing values per column after handling:")
      print(data.isnull().sum())
```

Missing values per column after handling: Туре 0 Days for shipping (real) 0 Days for shipment (scheduled) 0 Benefit per order 0 Sales per customer 0 Delivery Status 0 Late\_delivery\_risk 0 Category Id 0 Category Name 0 Customer City 0 Customer Country 0 Customer Email 0 Customer Fname 0 Customer Id 0 0 Customer Lname Customer Password 0

```
Customer Segment
     Customer State
                                        0
     Customer Street
                                        0
     Customer Zipcode
                                        0
     Department Id
                                        0
     Department Name
                                        0
     Latitude
                                        0
     Longitude
                                        0
     Market
                                        0
     Order City
                                        0
     Order Country
                                        0
     Order Customer Id
                                        0
                                        0
     order date (DateOrders)
                                        0
     Order Id
     Order Item Cardprod Id
                                        0
     Order Item Discount
                                        0
     Order Item Discount Rate
                                        0
     Order Item Id
                                        0
     Order Item Product Price
                                        0
     Order Item Profit Ratio
                                        0
     Order Item Quantity
                                        0
     Sales
                                        0
     Order Item Total
                                        0
     Order Profit Per Order
                                        0
     Order Region
                                        0
     Order State
                                        0
     Order Status
                                        0
     Product Card Id
                                        0
     Product Category Id
                                        0
     Product Image
                                        0
     Product Name
                                        0
     Product Price
                                        0
     Product Status
     shipping date (DateOrders)
                                        0
     Shipping Mode
                                        0
     dtype: int64
[66]: if data[col].dtype != 'object':
       data.corr()
      else:
       print("\ncannot perform co-relation")
```

0

cannot perform co-relation

### 8 Feature selection

```
[68]: from sklearn.feature_selection import SelectKBest, f_regression, f_classif, RFE from sklearn.linear_model import LinearRegression, Lasso, LogisticRegression from sklearn.ensemble import RandomForestRegressor, RandomForestClassifier from sklearn.preprocessing import LabelEncoder from sklearn.model_selection import train_test_split
```

```
[69]: # -----
     # Define Candidate Features for Each Target
     # -----
     # Based on domain knowledge and available variable names:
     # For Fulfillment Time ("Days for shipping (real)"):
     candidate_features_fulfillment = [
         "Days for shipment (scheduled)",
         "Shipping Mode",
         "Order Item Quantity",
         "Order Region",
         "Order State",
         "Order Country",
         "Latitude",
         "Longitude",
         "Customer City",
         "Customer State",
         "Market",
         "Order Status",
         "order date (DateOrders)",
         "shipping date (DateOrders)",
         "Product Category Id"
     ]
     # For Order Profit ("Order Profit Per Order"):
     candidate_features_profit = [
         "Order Item Product Price",
         "Order Item Discount Rate",
         "Order Item Quantity",
         "Benefit per order",
         "Order Item Profit Ratio",
         "Sales per customer",
         "Product Price",
         "Department Name",
         "Product Category Id",
         "Shipping Mode",
         "Order Region",
         "Customer Segment"
     ]
```

```
# For Delay ("Delivery Status"):
candidate_features_delay = [
    "Shipping Mode",
    "Days for shipment (scheduled)",
    "Late_delivery_risk",
    "Order Status",
    "Customer State",
    "Order Region",
    "Market",
    "order date (DateOrders)",
    "shipping date (DateOrders)",
    "Latitude",
    "Longitude",
    "Product Category Id",
    "Order Item Quantity",
    "Customer City"
]
# Define targets (make sure these match exactly the column names in your data)
target fulfillment = "Days for shipping (real)"
target_profit = "Order Profit Per Order"
target_delay = "Delivery Status" # Assumed binary (0 = on time, 1 = delayed)
```

```
[70]: # -----
     # Preprocessing: Encode Categorical Variables
     # -----
     # We'll encode candidate features using LabelEncoder for simplicity.
     def encode candidates(df, features):
         for col in features:
             if col in df.columns and df[col].dtype == 'object':
                 le = LabelEncoder()
                 df[col] = le.fit_transform(df[col])
         return df
     # Combine all candidate features
     all_candidate_features = list(set(candidate_features_fulfillment +__
      →candidate_features_profit + candidate_features_delay))
     data = encode_candidates(data, all_candidate_features)
     # Optionally, drop rows with missing values in any candidate features or
      \hookrightarrow targets.
     data = data.dropna(subset=all_candidate_features + [target_fulfillment,__
       →target_profit, target_delay])
```

```
# 1. Feature Selection for Fulfillment Time (Regression)
     # -----
     print("\n=== Feature Selection for Fulfillment Time ===")
     features_ft = [f for f in candidate_features_fulfillment if f in data.columns]
     X_ft = data[features_ft]
     y_ft = data[target_fulfillment]
     # -- a. Filter Method: SelectKBest (F-test)
     selector_ft = SelectKBest(score_func=f_regression, k='all')
     selector_ft.fit(X_ft, y_ft)
     ft_scores = pd.DataFrame({
         'Feature': features_ft,
         'F-score': selector_ft.scores_,
         'p-value': selector_ft.pvalues_
     })
     print("\nSelectKBest (F-test) scores for Fulfillment Time:")
     print(ft_scores.sort_values(by='F-score', ascending=False))
     # -- b. Wrapper Method: RFE with Linear Regression
     estimator_lr_ft = LinearRegression()
     rfe_ft = RFE(estimator_lr_ft, n_features_to_select=2) # Adjust the number to_
      ⇔select
     rfe_ft.fit(X_ft, y_ft)
     selected_rfe_ft = X_ft.columns[rfe_ft.support_]
     print("\nRFE selected features for Fulfillment Time:")
     print(list(selected_rfe_ft))
```

=== Feature Selection for Fulfillment Time ===

SelectKBest (F-test) scores for Fulfillment Time:

```
Feature
                                       F-score
                                                 p-value
0
   Days for shipment (scheduled) 65463.268997 0.000000
1
                   Shipping Mode 65386.909493 0.000000
11
                    Order Status
                                     12.999290 0.000312
                                      5.080094 0.024203
9
                  Customer State
         order date (DateOrders)
                                      4.927262 0.026437
12
4
                     Order State
                                      3.526612 0.060393
6
                        Latitude
                                      2.995160 0.083515
7
                       Longitude
                                      2.760773 0.096603
3
                    Order Region
                                      2.603879 0.106604
8
                   Customer City
                                      1.389426 0.238504
13
      shipping date (DateOrders)
                                      0.781335 0.376734
5
                   Order Country
                                      0.699623 0.402912
10
                          Market
                                      0.206219 0.649748
2
             Order Item Quantity
                                      0.118689 0.730461
```

10

11

RFE selected features for Fulfillment Time: ['Days for shipment (scheduled)', 'Shipping Mode']

```
# 2. Feature Selection for Profit (Regression)
     # -----
     print("\n=== Feature Selection for Profit ===")
     features_profit = [f for f in candidate_features_profit if f in data.columns]
     X_profit = data[features_profit]
     y_profit_val = data[target_profit]
     # -- a. Filter Method: SelectKBest (F-test)
     selector_profit = SelectKBest(score_func=f_regression, k='all')
     selector_profit.fit(X_profit, y_profit_val)
     profit_scores = pd.DataFrame({
         'Feature': features_profit,
         'F-score': selector profit.scores ,
         'p-value': selector_profit.pvalues_
     })
     print("\nSelectKBest (F-test) scores for Profit:")
     print(profit_scores.sort_values(by='F-score', ascending=False))
     # -- b. Wrapper Method: RFE with Linear Regression
     estimator_lr_profit = LinearRegression()
     rfe_profit = RFE(estimator_lr_profit, n_features_to_select=3) # Adjust as_
      \rightarrowneeded
     rfe_profit.fit(X_profit, y_profit_val)
     selected_rfe_profit = X_profit.columns[rfe_profit.support_]
     print("\nRFE selected features for Profit:")
     print(list(selected_rfe_profit))
```

=== Feature Selection for Profit ===

SelectKBest (F-test) scores for Profit:

Feature F-score p-value 4 Order Item Profit Ratio 3.809044e+05 0.000000e+00 5 Sales per customer 3.274803e+03 0.000000e+00 0 Order Item Product Price 1.953110e+03 0.000000e+00 6 Product Price 1.953110e+03 0.000000e+00 Product Category Id 1.837531e+02 7.700454e-42 8 1 Order Item Discount Rate 6.277077e+01 2.335309e-15 2 Order Item Quantity 4.448517e+01 2.570264e-11 7 Department Name 6.784693e+00 9.195040e-03

Order Region 2.180597e+00 1.397620e-01 Customer Segment 1.136508e+00 2.863928e-01

```
9
                   Shipping Mode 1.058673e+00 3.035193e-01
     3
               Benefit per order -1.270275e+19 1.000000e+00
     RFE selected features for Profit:
     ['Order Item Quantity', 'Benefit per order', 'Order Item Profit Ratio']
 []:
[73]: | # -----
     # 3. Feature Selection for Delay (Classification)
     # -----
     print("\n=== Feature Selection for Delay ===")
     features_delay = [f for f in candidate_features_delay if f in data.columns]
     X_delay = data[features_delay]
     y_delay_val = data[target_delay]
     # -- a. Filter Method: SelectKBest (F-test for classification)
     selector_delay = SelectKBest(score_func=f_classif, k='all')
     selector_delay.fit(X_delay, y_delay_val)
     delay_scores = pd.DataFrame({
         'Feature': features_delay,
         'F-score': selector_delay.scores_,
         'p-value': selector_delay.pvalues_
     })
     print("\nSelectKBest (F-test) scores for Delay:")
     print(delay_scores.sort_values(by='F-score', ascending=False))
     # -- b. Wrapper Method: RFE with Logistic Regression
     estimator_lr_delay = LogisticRegression(max_iter=1000, solver='liblinear')
     rfe_delay = RFE(estimator_lr_delay, n_features_to_select=2) # Adjust as needed
     rfe_delay.fit(X_delay, y_delay_val)
     selected_rfe_delay = X_delay.columns[rfe_delay.support_]
     print("\nRFE selected features for Delay:")
     print(list(selected_rfe_delay))
     === Feature Selection for Delay ===
     /opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/site-
     packages/sklearn/feature_selection/_univariate_selection.py:113: RuntimeWarning:
     divide by zero encountered in divide
       f = msb / msw
     SelectKBest (F-test) scores for Delay:
                             Feature
                                                        p-value
                                           F-score
     2
                   Late_delivery_risk
                                               inf 0.00000e+00
     1
        Days for shipment (scheduled) 1.513449e+04 0.000000e+00
     0
                        Shipping Mode 1.443895e+04 0.000000e+00
```

```
3
                    Order Status 5.091725e+01 6.933835e-33
5
                    Order Region 6.336798e+00 2.721722e-04
8
      shipping date (DateOrders) 4.784055e+00 2.463568e-03
                   Customer City 3.920796e+00 8.244400e-03
13
         order date (DateOrders) 3.462981e+00 1.553543e-02
7
9
                        Latitude 1.075386e+00 3.580560e-01
6
                          Market 9.175431e-01 4.313597e-01
4
                  Customer State 8.030894e-01 4.919134e-01
                       Longitude 7.142550e-01 5.433110e-01
10
12
             Order Item Quantity 4.583997e-01 7.113587e-01
             Product Category Id 3.061026e-01 8.210076e-01
11
```

RFE selected features for Delay:
['Shipping Mode', 'Late\_delivery\_risk']

#### 8.0.1 Summary on feature selection

From the test results as above and consdiering the domain knowledge For **fulfillment time**, all techniques agree that "Days for shipment (scheduled)" and "Shipping Mode" are the key predictors, while "Order Item Quantity" appears to add little value.

For Profit("Order Profit Per Order") There seems to be a strong signal from "Benefit per order", "Order Item Quantity" suggesting it is a dominant predictor of profit. "Order Item Profit Ratio" also appears relevant. However, you might want to investigate the extreme value seen for "Benefit per order" in the F-test results, as it might be due to outliers or data quality issues.

For **Delay** ("**Delivery Status**") "Late\_delivery\_risk" is consistently the most important feature for predicting delays. "Shipping Mode" and "Days for shipment (scheduled)" also contribute but to a lesser extent. "Order Status" might also add some signals.

```
[75]: data.columns
```

```
[75]: Index(['Type', 'Days for shipping (real)', 'Days for shipment (scheduled)',
             'Benefit per order', 'Sales per customer', 'Delivery Status',
             'Late_delivery_risk', 'Category Id', 'Category Name', 'Customer City',
             'Customer Country', 'Customer Email', 'Customer Fname', 'Customer Id',
             'Customer Lname', 'Customer Password', 'Customer Segment',
             'Customer State', 'Customer Street', 'Customer Zipcode',
             'Department Id', 'Department Name', 'Latitude', 'Longitude', 'Market',
             'Order City', 'Order Country', 'Order Customer Id',
             'order date (DateOrders)', 'Order Id', 'Order Item Cardprod Id',
             'Order Item Discount', 'Order Item Discount Rate', 'Order Item Id',
             'Order Item Product Price', 'Order Item Profit Ratio',
             'Order Item Quantity', 'Sales', 'Order Item Total',
             'Order Profit Per Order', 'Order Region', 'Order State', 'Order Status',
             'Product Card Id', 'Product Category Id', 'Product Image',
             'Product Name', 'Product Price', 'Product Status',
             'shipping date (DateOrders)', 'Shipping Mode'],
            dtype='object')
```

```
[76]: # -----
     # Feature Selection based on previous analysis:
     # For Fulfillment Time, Profit, and Delay we select:
     selected_features = [
         'Days for shipment (scheduled)',
         'Shipping Mode',
         'Benefit per order',
         'Order Item Quantity',
         'Order Item Profit Ratio',
         'Late_delivery_risk'
     target_features = [
         'Days for shipping (real)', # Fulfillment Time
         'Order Profit Per Order', # \mathit{Order\ Profit}
         'Delivery Status'
                                       # Likelihood of Delay
     ]
```

```
[77]: # Create a new DataFrame with the selected features and targets

df_q4 = data[selected_features + target_features].dropna()

print("Data shape after dropping missing values:", df_q4.shape)
```

Data shape after dropping missing values: (180519, 9)

```
[78]: # -----
      # Categorical Feature Encoding
      # Encode "Shipping Mode" (assumed categorical)
     le = LabelEncoder()
     df_q4['Shipping Mode'] = le.fit_transform(df_q4['Shipping Mode'])
      # Convert "Delivery Status" to Numeric
      # Check the type of "Delivery Status" and map if necessary.
     if df_q4['Delivery Status'].dtype == object:
         # Define a mapping. Adjust keys if your strings differ.
         mapping = {"On Time": 0, "Late delivery": 1}
         df_q4['Delivery Status'] = df_q4['Delivery Status'].map(mapping)
      # Drop any rows that might have become NaN after mapping (if there were,
      →unexpected values)
     df_q4 = df_q4.dropna(subset=['Delivery Status'])
     df_q4['Delivery Status'] = pd.to_numeric(df_q4['Delivery Status'],_
      →errors='coerce')
     print("Delivery Status type after conversion:", df_q4['Delivery Status'].dtype)
```

Delivery Status type after conversion: float64

Training set shape: (79181, 9) Test set shape: (19796, 9)

```
# (b) Model Implementation
     # Define the multi-head regression model in PyTorch
     class MultiHeadRegressionModel(nn.Module):
         def __init__(self, input_dim, hidden_dim=64):
             super(MultiHeadRegressionModel, self).__init__()
             # Shared feature extractor
             self.shared = nn.Sequential(
                nn.Linear(input_dim, hidden_dim),
                nn.ReLU(),
                nn.Linear(hidden_dim, hidden_dim),
                nn.ReLU()
             # Output head for Fulfillment Time Prediction (linear output)
             self.head_time = nn.Linear(hidden_dim, 1)
             # Output head for Order Profit Prediction (linear output)
             self.head_profit = nn.Linear(hidden_dim, 1)
             # Output head for Likelihood of Delay (binary classification;
       →BCEWithLogitsLoss applies sigmoid)
             self.head_delay = nn.Linear(hidden_dim, 1)
         def forward(self, x):
             features = self.shared(x)
             out_time = self.head_time(features)
             out_profit = self.head_profit(features)
             out_delay = self.head_delay(features) # raw logits; sigmoid will be_
       →applied in loss function
```

```
# Determine input dimension (number of selected features)
     input_dim = len(selected_features)
     model = MultiHeadRegressionModel(input_dim=input_dim, hidden_dim=64)
[81]: import torch
     import torch.nn as nn
     import torch.optim as optim
     # Print model architecture and total trainable parameters
     print(model)
     total_params = sum(p.numel() for p in model.parameters() if p.requires grad)
     print("Total trainable parameters:", total_params)
     # Loss functions:
     criterion time = nn.MSELoss()
                                            # For Fulfillment Time (regression)
     criterion_profit = nn.MSELoss() # For Order Profit (regression)
     criterion_delay = nn.BCEWithLogitsLoss() # For Likelihood of Delay (binary_
       \hookrightarrow classification)
     # Optimizer
     optimizer = optim.Adam(model.parameters(), lr=0.001)
     MultiHeadRegressionModel(
       (shared): Sequential(
         (0): Linear(in_features=6, out_features=64, bias=True)
         (1): ReLU()
         (2): Linear(in_features=64, out_features=64, bias=True)
         (3): ReLU()
       )
       (head_time): Linear(in_features=64, out_features=1, bias=True)
       (head_profit): Linear(in_features=64, out_features=1, bias=True)
       (head_delay): Linear(in_features=64, out_features=1, bias=True)
     Total trainable parameters: 4803
# (c) Training and Evaluation
     # Convert training data to PyTorch tensors
     X_train = torch.tensor(train_df[selected_features].values, dtype=torch.float32)
     y_train_time = torch.tensor(train_df['Days for shipping (real)'].values, __

dtype=torch.float32).view(-1, 1)
     y_train_profit = torch.tensor(train_df['Order Profit Per Order'].values,_

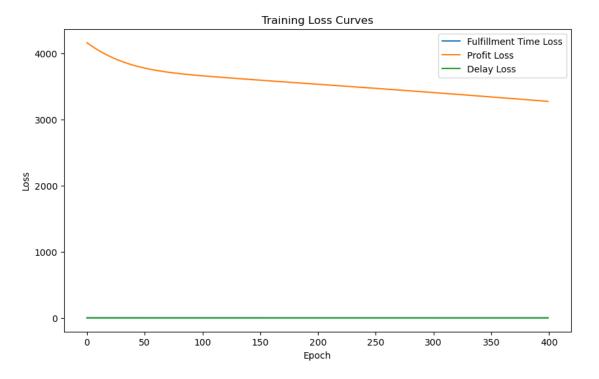
dtype=torch.float32).view(-1, 1)
```

return out\_time, out\_profit, out\_delay

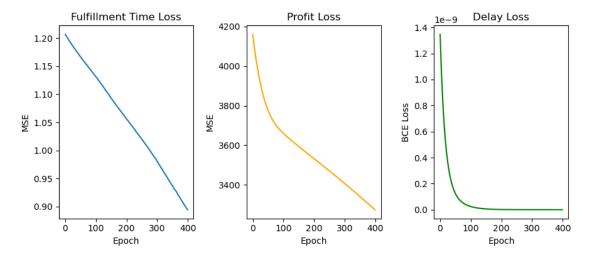
```
y_train_delay = torch.tensor(train_df['Delivery Status'].values.astype(np.
        →float32), dtype=torch.float32).view(-1, 1)
       # Convert test data to PyTorch tensors
       X_test = torch.tensor(test_df[selected_features].values, dtype=torch.float32)
       y test time = test df['Days for shipping (real)'].values
       y_test_profit = test_df['Order Profit Per Order'].values
       y_test_delay = test_df['Delivery Status'].values
[92]: # Training loop
      num epochs = 100
       loss_history_time = []
       loss history profit = []
       loss_history_delay = []
       model.train()
[92]: MultiHeadRegressionModel(
         (shared): Sequential(
           (0): Linear(in_features=6, out_features=64, bias=True)
           (1): ReLU()
           (2): Linear(in_features=64, out_features=64, bias=True)
           (3): ReLU()
         (head_time): Linear(in_features=64, out_features=1, bias=True)
         (head_profit): Linear(in_features=64, out_features=1, bias=True)
         (head_delay): Linear(in_features=64, out_features=1, bias=True)
       )
[100]: for epoch in range(num_epochs):
           optimizer.zero_grad()
           # Forward pass
           pred_time, pred_profit, pred_delay = model(X_train)
           # Compute losses for each output head
           loss_time = criterion_time(pred_time, y_train_time)
           loss_profit = criterion_profit(pred_profit, y_train_profit)
           loss_delay = criterion_delay(pred_delay, y_train_delay)
           total_loss = loss_time + loss_profit + loss_delay
           total_loss.backward()
           optimizer.step()
           loss_history_time.append(loss_time.item())
           loss_history_profit.append(loss_profit.item())
           loss_history_delay.append(loss_delay.item())
```

```
Epoch 10/100 | Time Loss: 0.9729 | Profit Loss: 3395.0505 | Delay Loss: 0.00 Epoch 20/100 | Time Loss: 0.9640 | Profit Loss: 3381.9282 | Delay Loss: 0.00 Epoch 30/100 | Time Loss: 0.9553 | Profit Loss: 3368.7456 | Delay Loss: 0.00 Epoch 40/100 | Time Loss: 0.9464 | Profit Loss: 3355.4766 | Delay Loss: 0.00 Epoch 50/100 | Time Loss: 0.9376 | Profit Loss: 3342.1084 | Delay Loss: 0.00 Epoch 60/100 | Time Loss: 0.9293 | Profit Loss: 3328.6497 | Delay Loss: 0.00 Epoch 70/100 | Time Loss: 0.9203 | Profit Loss: 3315.1208 | Delay Loss: 0.00 Epoch 80/100 | Time Loss: 0.9118 | Profit Loss: 3301.5249 | Delay Loss: 0.00 Epoch 90/100 | Time Loss: 0.9031 | Profit Loss: 3287.8542 | Delay Loss: 0.00 Epoch 100/100 | Time Loss: 0.8946 | Profit Loss: 3274.0740 | Delay Loss: 0.00
```

```
[102]: # Plot training loss curves
plt.figure(figsize=(10, 6))
plt.plot(loss_history_time, label="Fulfillment Time Loss")
plt.plot(loss_history_profit, label="Profit Loss")
plt.plot(loss_history_delay, label="Delay Loss")
plt.xlabel("Epoch")
plt.ylabel("Loss")
plt.title("Training Loss Curves")
plt.legend()
plt.show()
```

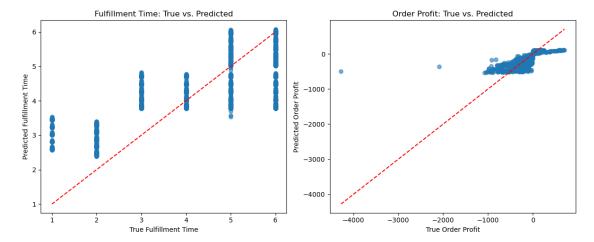


```
[104]: plt.figure(figsize=(12, 4))
       plt.subplot(1, 4, 1)
       plt.plot(loss_history_time, label='Time Loss')
       plt.title("Fulfillment Time Loss")
       plt.xlabel("Epoch")
       plt.ylabel("MSE")
       plt.subplot(1, 4, 2)
       plt.plot(loss_history_profit, label='Profit Loss', color='orange')
       plt.title("Profit Loss")
       plt.xlabel("Epoch")
       plt.ylabel("MSE")
       plt.subplot(1, 4, 3)
       plt.plot(loss_history_delay, label='Delay Loss', color='green')
       plt.title("Delay Loss")
       plt.xlabel("Epoch")
       plt.ylabel("BCE Loss")
       plt.tight_layout()
       plt.show()
```



```
[106]: # Evaluation on the test dataset
    model.eval()
    with torch.no_grad():
        pred_time_test, pred_profit_test, pred_delay_test = model(X_test)
```

```
pred_time_test = pred_time_test.numpy().flatten()
           pred_profit_test = pred_profit_test.numpy().flatten()
           # Apply sigmoid to the delay logits to get probability estimates
           pred_delay_test_prob = torch.sigmoid(pred_delay_test).numpy().flatten()
[108]: from sklearn.metrics import r2_score, mean_squared_error, mean_absolute_error
       # Compute evaluation metrics for regression outputs
       mae_time = mean_absolute_error(y_test_time, pred_time_test)
       r2_time = r2_score(y_test_time, pred_time_test)
       mae_profit = mean_absolute_error(y_test_profit, pred_profit_test)
       r2_profit = r2_score(y_test_profit, pred_profit_test)
       print("\n--- Model Evaluation ---")
       print(f"Fulfillment Time - MAE: {mae_time:.4f}, R2: {r2_time:.4f}")
       print(f"Order Profit - MAE: {mae_profit:.4f}, R2: {r2_profit:.4f}")
      --- Model Evaluation ---
      Fulfillment Time - MAE: 0.7629, R<sup>2</sup>: 0.6949
      Order Profit - MAE: 29.8855, R2: 0.6809
[110]: # Compute BCE loss on the test set for delay
       y_test_delay_tensor = torch.tensor(y_test_delay.astype(np.float32), dtype=torch.
        \hookrightarrowfloat32).view(-1, 1)
       bce_loss_test = criterion_delay(pred_delay_test, y_test_delay_tensor)
       print(f"Delay Prediction - BCE Loss: {bce_loss_test.item():.4f}")
      Delay Prediction - BCE Loss: 0.0000
[112]: # Scatter plots: True vs. Predicted for Fulfillment Time and Order Profit
      plt.figure(figsize=(12, 5))
       plt.subplot(1, 2, 1)
       plt.scatter(y_test_time, pred_time_test, alpha=0.6)
       plt.xlabel("True Fulfillment Time")
       plt.ylabel("Predicted Fulfillment Time")
       plt.title("Fulfillment Time: True vs. Predicted")
       plt.plot([min(y_test_time), max(y_test_time)], [min(y_test_time),__
        →max(y_test_time)], 'r--')
       plt.subplot(1, 2, 2)
       plt.scatter(y_test_profit, pred_profit_test, alpha=0.6)
       plt.xlabel("True Order Profit")
       plt.ylabel("Predicted Order Profit")
       plt.title("Order Profit: True vs. Predicted")
```



[]:	
Г 1.	

# $ML_HW4$

February 19, 2025

## 1 Question 2: Image Compression using PCA

```
[2]: from PIL import Image import numpy as np from numpy.linalg import eig import matplotlib.pyplot as plt
```

[3]: image = Image.open('tiger.jpg')
image

[3]:



```
[4]: # Convert the image to a numpy array (RGB)
     img_array = np.array(image)
     img_array
[4]: array([[[ 20,
                    16, 15],
             [ 20,
                    16,
                         15],
             [ 18,
                    17, 13],
             [138, 116, 103],
             [138, 116, 103],
             [138, 116, 103]],
            [[ 20, 16, 15],
             [ 19, 15, 14],
             [ 17, 16, 12],
             [139, 117, 104],
             [139, 117, 104],
             [139, 117, 104]],
            [[ 19, 15, 14],
             [ 19,
                   15, 14],
             [ 17,
                   16, 12],
             [140, 118, 105],
             [140, 118, 105],
             [140, 118, 105]],
            ...,
            [[186, 145, 91],
             [194, 154, 102],
             [193, 156, 104],
             [121, 113, 111],
             [114, 109, 113],
             [107, 106, 111]],
            [[170, 131, 76],
             [177, 138, 83],
             [185, 148, 95],
             [118, 110, 108],
             [113, 108, 112],
             [107, 106, 111]],
            [[186, 147, 90],
```

```
[180, 144, 86],
              [180, 145, 89],
              [140, 132, 130],
              [134, 129, 133],
              [124, 123, 128]]], dtype=uint8)
 [5]: img_array.shape
 [5]: (900, 1200, 3)
 [6]: # Store all the three matrices into separate variables
      red = img_array[:, :, 0]
      green = img_array[:, :, 1]
      blue = img_array[:, :, 2]
 [7]: red
 [7]: array([[ 20, 20, 18, ..., 138, 138, 138],
             [ 20, 19, 17, ..., 139, 139, 139],
             [ 19, 19, 17, ..., 140, 140, 140],
             [186, 194, 193, ..., 121, 114, 107],
             [170, 177, 185, ..., 118, 113, 107],
             [186, 180, 180, ..., 140, 134, 124]], dtype=uint8)
 [8]: red.shape
 [8]: (900, 1200)
 [9]: # There are 900 rows with 1200 columns
[10]: # Now use PCA on all three matrices to compress the data. The reduced matrix
      # can be obtained by dropping the columns corresponding to the smaller
      # eigen-values
[11]: # Calculate covariance matrices
      cov_red = np.cov(red.T)
      cov_green = np.cov(green.T)
      cov_blue = np.cov(blue.T)
[12]: # Get eigenvalues and eigenvectors
      eigenvalues_red, eigenvectors_red = eig(cov_red)
      eigenvalues_green, eigenvectors_green = eig(cov_green)
      eigenvalues_blue, eigenvectors_blue = eig(cov_blue)
```

```
[13]: print(eigenvalues_red.shape)
      print(eigenvectors_red.shape)
     (1200,)
     (1200, 1200)
[14]: # Sort eigenvalues and eigenvectors in descending order
      idx_red = eigenvalues_red.argsort()[::-1]
      eigenvalues_red = eigenvalues_red[idx_red]
      eigenvectors_red = eigenvectors_red[:, idx_red]
      idx_green = eigenvalues_green.argsort()[::-1]
      eigenvalues_green = eigenvalues_green[idx_green]
      eigenvectors_green = eigenvectors_green[:, idx_green]
      idx_blue = eigenvalues_blue.argsort()[::-1]
      eigenvalues_blue = eigenvalues_blue[idx_blue]
      eigenvectors_blue = eigenvectors_blue[:, idx_blue]
[15]: #Just to test the approach, taking k as 50
      k = 50
      eigenvectors_red_reduced = eigenvectors_red[:, :k]
      eigenvectors green reduced = eigenvectors green[:, :k]
      eigenvectors_blue_reduced = eigenvectors_blue[:, :k]
      # Project data onto reduced eigenvector space
      projected_red = red @ eigenvectors_red_reduced
      projected_green = green @ eigenvectors_green_reduced
      projected_blue = blue @ eigenvectors_blue_reduced
      # Reconstruct the compressed image channels
      reconstructed_red = (projected_red @ eigenvectors_red_reduced.T).reshape(red.
       ⇔shape)
      reconstructed_green = (projected_green @ eigenvectors_green_reduced.T).
       ⇔reshape(green.shape)
      reconstructed_blue = (projected_blue @ eigenvectors_blue_reduced.T).
       →reshape(blue.shape)
      # Ensure values are in valid range (0-255)
      reconstructed_red = np.clip(reconstructed_red, 0, 255)
      reconstructed_green = np.clip(reconstructed_green, 0, 255)
      reconstructed_blue = np.clip(reconstructed_blue, 0, 255)
      # Convert back to uint8
      reconstructed_red = reconstructed_red.astype(np.uint8)
```

```
reconstructed_green = reconstructed_green.astype(np.uint8)
      reconstructed_blue = reconstructed_blue.astype(np.uint8)
     /tmp/ipykernel_1691/2698842910.py:25: ComplexWarning: Casting complex values to
     real discards the imaginary part
       reconstructed_red = reconstructed_red.astype(np.uint8)
     /tmp/ipykernel_1691/2698842910.py:26: ComplexWarning: Casting complex values to
     real discards the imaginary part
       reconstructed_green = reconstructed_green.astype(np.uint8)
     /tmp/ipykernel_1691/2698842910.py:27: ComplexWarning: Casting complex values to
     real discards the imaginary part
       reconstructed_blue = reconstructed_blue.astype(np.uint8)
[16]: | print(eigenvectors_red_reduced.shape)
      print(projected_red.shape)
      print(reconstructed_red.shape)
     (1200, 50)
     (900, 50)
     (900, 1200)
[17]: compressed_image = np.stack([
          reconstructed_red,
          reconstructed_green,
         reconstructed_blue
      ], axis=2)
      compressed_img = Image.fromarray(compressed_image)
[18]: # Save the new image and note the size
      compressed_img
「18]:
```

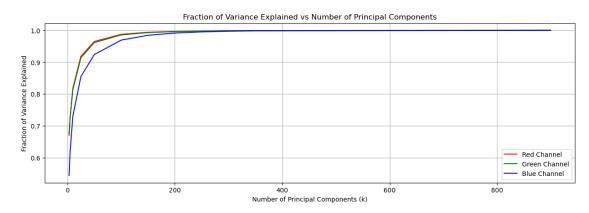


```
[19]: # Choose k [3, 5, 10, 25, 50, 100,
      # 150, 200, 250, 300, 350, p] where p is all the principal components
      k_values = [3, 5, 10, 25, 50, 100, 150, 200, 250, 300, 350]
      p = red.shape[0]
      k_values.append(p)
      # Initialize lists to store results
      compression_ratios = []
      variance_fractions_red = []
      variance_fractions_green = []
      variance_fractions_blue = []
      image_sizes = []
      original_size = red.size + green.size + blue.size
      for k in k_values:
          # Reduce dimensionality
          eigenvectors_red_reduced = eigenvectors_red[:, :k]
          eigenvectors_green_reduced = eigenvectors_green[:, :k]
          eigenvectors_blue_reduced = eigenvectors_blue[:, :k]
```

```
# Project data
         projected_red = red @ eigenvectors_red_reduced
         projected_green = green @ eigenvectors_green_reduced
         projected_blue = blue @ eigenvectors_blue_reduced
          # Calculate compressed size
          compressed_size = (projected_red.size + eigenvectors_red_reduced.size +
                           projected_green.size + eigenvectors_green_reduced.size +
                           projected_blue.size + eigenvectors_blue_reduced.size)
         print("K value: ", k, "compressed_size: ", compressed_size, "original_size:__
       →", original_size)
          # Calculate compression ratio
         ratio = compressed_size/original_size
          compression_ratios.append(ratio)
          # Calculate variance fractions
         var_red = np.sum(eigenvalues_red[:k]) / np.sum(eigenvalues_red)
         var_green = np.sum(eigenvalues_green[:k]) / np.sum(eigenvalues_green)
         var_blue = np.sum(eigenvalues_blue[:k]) / np.sum(eigenvalues_blue)
         variance_fractions_red.append(var_red)
         variance_fractions_green.append(var_green)
         variance_fractions_blue.append(var_blue)
     K value: 3 compressed size: 18900 original size: 3240000
     K value: 5 compressed_size: 31500 original_size: 3240000
     K value: 10 compressed_size: 63000 original_size: 3240000
     K value: 25 compressed_size: 157500 original_size: 3240000
     K value: 50 compressed_size: 315000 original_size: 3240000
     K value: 100 compressed_size: 630000 original_size: 3240000
     K value: 150 compressed_size: 945000 original_size: 3240000
     K value: 200 compressed size: 1260000 original size: 3240000
     K value: 250 compressed_size: 1575000 original_size:
                                                            3240000
     K value: 300 compressed size: 1890000 original size: 3240000
     K value: 350 compressed_size: 2205000 original_size: 3240000
     K value: 900 compressed_size: 5670000 original_size: 3240000
[20]: # Plot the fraction of variance as k increases
     plt.figure(figsize=(15, 10))
     plt.subplot(2, 1, 1)
     plt.plot(k_values, variance_fractions_red, 'r-', label='Red Channel')
     plt.plot(k_values, variance_fractions_green, 'g-', label='Green Channel')
     plt.plot(k_values, variance_fractions_blue, 'b-', label='Blue Channel')
     plt.xlabel('Number of Principal Components (k)')
```

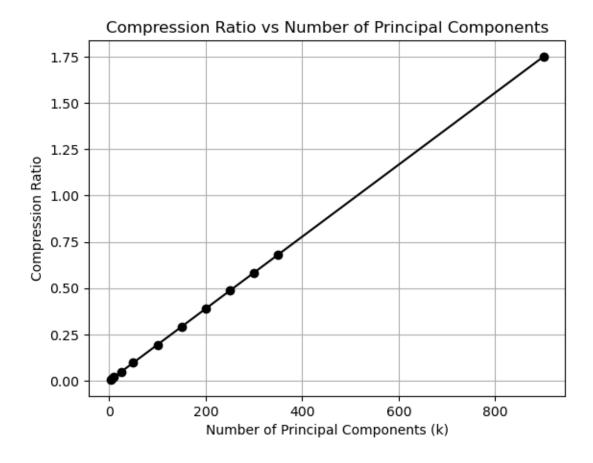
```
plt.ylabel('Fraction of Variance Explained')
plt.title('Fraction of Variance Explained vs Number of Principal Components')
plt.legend()
plt.grid(True)
```

/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/site-packages/matplotlib/cbook.py:1699: ComplexWarning: Casting complex values to real discards the imaginary part return math.isfinite(val)
/opt/conda/envs/anaconda-2024.02-py310/lib/python3.10/site-packages/matplotlib/cbook.py:1345: ComplexWarning: Casting complex values to real discards the imaginary part return np.asarray(x, float)



```
[21]: # Plot the compression ratio (size of the new image/ size of # original image) as a function of k where k is the number of principal → components # used to construct the compressed image
```

```
[22]: # Plot 2: Compression Ratio
plt.plot(k_values, compression_ratios, 'k-', marker='o')
plt.xlabel('Number of Principal Components (k)')
plt.ylabel('Compression Ratio')
plt.title('Compression Ratio vs Number of Principal Components')
plt.grid(True)
plt.show()
```



```
[23]: print("\nDetailed Results:\n")
   print("k\tVariance Fraction (R,G,B)\t\tCompression Ratio")
   print("-" * 70)
   for i, k in enumerate(k_values):
        print(f"{k}\t({variance_fractions_red[i]:.3f}, {variance_fractions_green[i]:
        -.3f}, {variance_fractions_blue[i]:.3f})\t{compression_ratios[i]:.4f}")
```

#### Detailed Results:

k	Variance Fraction (R,G,B)	Compression Ratio	
3	(0.670-0.000j, 0.676-0.000j	, 0.544-0.000j)	
5	(0.728-0.000j, 0.727-0.000j	, 0.620-0.000j) 0.0097	
10	(0.818-0.000j, 0.813-0.000j	, 0.730-0.000j) 0.0194	
25	(0.918-0.000j, 0.913-0.000j	, 0.855-0.000j) 0.0486	
50	(0.965-0.000j, 0.961-0.000j	, 0.924-0.000j) 0.0972	
100	(0.987-0.000j, 0.985-0.000j	, 0.969-0.000j) 0.1944	
150	(0.994-0.000j, 0.993-0.000j	, 0.984-0.000j) 0.2917	
200	(0.997-0.000j, 0.996-0.000j	, 0.991-0.000j) 0.3889	

```
(0.998-0.000j, 0.998-0.000j, 0.995-0.000j)
     300
             (0.999-0.000j, 0.999-0.000j, 0.997-0.000j)
                                                              0.5833
             (0.999-0.000j, 0.999-0.000j, 0.998-0.000j)
     350
                                                              0.6806
     900
             (1.000-0.000j, 1.000-0.000j, 1.000-0.000j)
                                                              1.7500
[24]: # Approach 2
      # Using PCA Package
[25]: import numpy as np
      import matplotlib.pyplot as plt
      from sklearn.decomposition import PCA
      from imageio import imread
      red = img_array[:, :, 0]
      green = img array[:, :, 1]
      blue = img_array[:, :, 2]
      def apply_pca(channel, k):
          h, w = channel.shape
          channel_reshaped = channel.reshape(h, w)
          pca = PCA(n_components=k)
          transformed = pca.fit_transform(channel_reshaped)
          reconstructed = pca.inverse_transform(transformed)
          return reconstructed, pca.explained_variance_ratio_
      k values = [3, 5, 10, 25, 50, 100, 150, 200, 250, 300]
      p = red.shape[0]
      k values.append(p)
      for k in k values:
          red_compressed, var_red = apply_pca(red, k)
          green_compressed, var_green = apply_pca(green, k)
          blue_compressed, var_blue = apply_pca(blue, k)
          compressed img = np.stack([red_compressed, green_compressed,_
       ⇒blue_compressed], axis=2)
          # Clip and convert to uint8
          compressed_img = np.clip(compressed_img, 0, 255).astype(np.uint8)
          # Display one of the compressed images
          if k in [10, 50, 100, 300]:
              plt.figure(figsize=(3, 5))
              plt.imshow(compressed_img)
              plt.title(f"PCA Compression with {k} Components")
```

0.4861

250

plt.axis('off')
plt.show()

PCA Compression with 10 Components



PCA Compression with 50 Components



PCA Compression with 100 Components



### PCA Compression with 300 Components



### 2 Question 3: Feed-Forward neural network

```
[27]: import numpy as np
      def sigmoid(z):
          return 1 / (1 + np.exp(-z))
     x1 = 0
     x2 = 1
      w_h1_bias, w_h1_x1, w_h1_x2 = 2.5, 2, 1.5
      w_h2_bias, w_h2_x1, w_h2_x2 = 1.5, -2, -1
     w_y_h1, w_y_h2 = -2, 2, 1
      b_h = 1
      b_y = 1
      # Forward propagation
      z_h1 = w_h1_bias * b_h + w_h1_x1 * x1 + w_h1_x2 * x2
     h1 = sigmoid(z_h1)
      z_h2 = w_h2_bias * b_h + w_h2_x1 * x1 + w_h2_x2 * x2
     h2 = sigmoid(z_h2)
      z_y = w_y_{bias} * b_y + w_y_{h1} * h1 + w_y_{h2} * h2
      0 = sigmoid(z_y)
```

[28]: # Calculate the output values at nodes h1, h2, and  $\hat{y}$  of this network for input

```
print("Output value at node h1: ", round(h1, 3))
      print("Output value at node h2: ", round(h2, 3))
      print("Output value at node y: ", round(0, 3))
     Output value at node h1: 0.982
     Output value at node h2: 0.622
     Output value at node y: 0.643
[29]: y_target = 1
      error = 0.5 * (y_target - 0) ** 2
      error
[29]: 0.06388215053115195
[30]: def sigmoid_derivative(z):
          return z * (1 - z)
[31]: # Backpropagation
      # assume the learning rate is =0.1
      alpha = 0.1
      delta_y = (0 - y_target) * sigmoid_derivative(0)
      delta_h1 = delta_y * w_y_h1 * sigmoid_derivative(h1)
      delta_h2 = delta_y * w_y_h2 * sigmoid_derivative(h2)
[32]: print(delta_h1)
      print(delta_h2)
      print(delta_y)
     -0.0029000771766557834
     -0.01929287884753416
     -0.08209605995918927
[33]: # Update weights
      # the three incoming weights to node h1
      w_h1_bias = (w_h1_bias) - (alpha * delta_h1 * b_h)
      w_h1_x1 = (w_h1_x1) - (alpha * delta_h1 * x1)
      w_h1_x2 = (w_h1_x2) - (alpha * delta_h1 * x2)
      # the three incoming weights to node h2
      w_h2_bias = (w_h2_bias) - (alpha * delta_h2 * b_h)
      w_h2_x1 = (w_h2_x1) - (alpha * delta_h2 * x1)
      w_h2_x2 = (w_h2_x2) - (alpha * delta_h2 * x2)
      # and the three incoming weights to node \hat{y}
```

```
w_y_bias = (w_y_bias) - (alpha * delta_y * b_y)
      w_y_h1 = (w_y_h1) - (alpha * delta_y * h1)
      w_y_h2 = (w_y_h2) - (alpha * delta_y * h2)
[34]: print("Updated Weights:")
      print("w_h1_bias: ", round(w_h1_bias, 3), "w_h1_x1: ", round(w_h1_x1, 3),__
      \rightarrow"w_h1_x2: ", round(w_h1_x2, 3))
      print("w_h2_bias: ", round(w_h2_bias, 3), "w_h2_x1: ", round(w_h2_x1, 3),__
      \rightarrow"w_h2_x2: ", round(w_h2_x2, 3))
      print("w_y_bias: ", round(w_y_bias, 3), "w_y_h1: ", round(w_y_h1, 3), "w_y_h2:__
       \rightarrow", round(w_y_h2, 3))
     Updated Weights:
     w_h1_bias: 2.5 w_h1_x1: 2.0 w_h1_x2: 1.5
     w_h2_bias: 1.502 w_h2_x1: -2.0 w_h2_x2: -0.998
     w_y_bias: -1.992 w_y_h1: 2.008 w_y_h2: 1.005
 []:
 []:
```