

Lab1_FFNN

November 4, 2025

1 Laboratory 1 — Feed Forward Neural Networks (FFNN)

This notebook implements the first lab of the *AI and Cybersecurity* course.

It follows the official brief (`resources/Lab1_FFNN.txt`) and develops a full **Machine Learning pipeline** using PyTorch to explore, train, and evaluate Feed Forward Neural Networks on the CICIDS2017 dataset.

This lab is organized into tasks:

- Task 1: Data preprocessing (cleaning, splitting, outliers, normalization)
- Task 2: Shallow NN (1 layer), train sizes {32, 64, 128}, metrics and analysis; then ReLU change
- Task 3: Impact of specific features (Destination Port), bias test and port removal
- Task 4: Loss function impact (weighted CrossEntropy)
- Task 5: Deep NN, batch size, optimizer comparisons
- Task 6: Overfitting and regularization (dropout, batchnorm, weight decay)

1.1 Setup

```
[1]: import sys
print(sys.executable)
print(sys.version)

/Users/elainnocenti/Documents/Projects/LaTeX/AImSecure/venv/bin/python3.14
3.14.0 (main, Oct 7 2025, 09:34:52) [Clang 17.0.0 (clang-1700.3.19.1)]
```

```
[2]: # --- Import libraries ---
import os
import time
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import json

from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler, MinMaxScaler, RobustScaler, □
    ↵LabelEncoder
from sklearn.utils.class_weight import compute_class_weight
from sklearn.metrics import classification_report, confusion_matrix, □
    ↵accuracy_score, f1_score
```

```
import torch
import torch.nn as nn
import torch.optim as optim
from torch.utils.data import Dataset, DataLoader, TensorDataset
```

1.1.1 Device Settings

```
[3]: device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
device = "cpu"
print(f"The device is set to: {device}")
```

The device is set to: cpu

1.1.2 Paths setup

```
[4]: # --- Define Paths ---
project_path = '../'
data_path = project_path + 'data/'
results_path = project_path + 'results/'

# Ensure directories exist
os.makedirs(project_path, exist_ok=True)
os.makedirs(data_path, exist_ok=True)
os.makedirs(results_path, exist_ok=True)

print(f"Project path: {project_path}")
print(f"Data path: {data_path}")
print(f"Results path: {results_path}")
```

Project path: ../
Data path: ../data/
Results path: ../results/

```
[5]: # --- Set visual style ---
sns.set(style="whitegrid", palette="muted", font_scale=1.1)

def save_plot(fig: plt.Figure, filename: str, path: str = "./plots/", fmt: str
             ↪= "png", dpi: int = 300, close_fig: bool = False) -> None:
    """
    Save a Matplotlib figure in a specific directory.

    Args:
        fig (plt.Figure): Matplotlib figure object to save.
        filename (str): Name of the file to save (e.g., 'plot.png').
        path (str, optional): Directory path to save the figure. Defaults to './
                             ↪plots/'.
        fmt (str, optional): File format for the saved figure. Defaults to
                            ↪'png'.
```

```

    dpi (int, optional): Dots per inch for the saved figure. Defaults to
    ↪300.

    Returns:
        None
    """
    # Ensure the directory exists
    os.makedirs(path, exist_ok=True)
    save_path = os.path.join(path, f"{filename}.{fmt}")

    # Save the figure
    fig.savefig(save_path, bbox_inches='tight', pad_inches=0.1, dpi=dpi, ↪
    ↪format=fmt)
    # plt.close(fig) # Removed to display plots in notebook

    if close_fig:
        plt.close(fig)

    print(f"Saved plot: {save_path}")

```

1.2 Task 1 — Data preprocessing

In this task, we prepare the dataset and ensure proper data quality and normalization before training.

We will:

- Load the dataset from `lab/data/dataset_lab_1.csv`.
- Inspect basic statistics, feature ranges, and class distribution.
- Remove missing values and duplicates (report before/after counts).
- Split the data into **train / validation / test (60% / 20% / 20%)**, using a fixed random seed for reproducibility.
- Perform **outlier analysis** (e.g., KDE, Z-score, IQR) and decide on an appropriate **scaling method**.
- Fit the scaler on the training data only and apply it to validation and test splits.

```
[6]: # --- Load dataset and perform initial inspection ---

# Set random seed for reproducibility
np.random.seed(42)

# Create directory for plots
save_dir = results_path + 'images/' + 'task1_plots/'
os.makedirs(save_dir, exist_ok=True)

# Load Dataset
file_path = data_path + 'dataset_lab_1.csv'
df = pd.read_csv(file_path)

# Basic info
print("Shape (raw):", df.shape)
print("Columns:", list(df.columns))
```

```
print("\nLabel distribution (raw):")
print(df['Label'].value_counts(dropna=False))
```

Shape (raw): (31507, 17)
Columns: ['Flow Duration', 'Flow IAT Mean', 'Fwd PSH Flags', 'Bwd Packet Length Mean', 'Bwd Packet Length Max', 'Flow Bytes/s', 'Down/Up Ratio', 'SYN Flag Count', 'Fwd Packet Length Mean', 'Fwd IAT Std', 'Packet Length Mean', 'Fwd Packet Length Max', 'Subflow Fwd Packets', 'Flow Packets/s', 'Total Fwd Packets', 'Destination Port', 'Label']

Label distribution (raw):

Label
Benign 20000
DoS Hulk 5000
PortScan 5000
Brute Force 1507
Name: count, dtype: int64

[7]: df

```
[7]:      Flow Duration  Flow IAT Mean  Fwd PSH Flags  Bwd Packet Length Mean \
0          303376     3.033760e+04           0             749.4
1            117     1.170000e+02           0              0.0
2            142     1.420000e+02           0              0.0
3            191     6.366667e+01           0             52.0
4              4     4.000000e+00           0              0.0
...
31502      5710955    1.903652e+06           0              0.0
31503      5862561    1.954187e+06           0              0.0
31504      5854872    1.951624e+06           0              0.0
31505      5555547    1.851849e+06           0              0.0
31506      5018204    1.672735e+06           0              0.0

      Bwd Packet Length Max  Flow Bytes/s  Down/Up Ratio  SYN Flag Count \
0            1448        12743.263           0              0
1              0         0.000             1              0
2              0         84507.040           0              0
3              52         921465.940           1              0
4              0        3000000.000           0              0
...
31502          ...          ...           ...           ...
31503          ...          ...           ...           ...
31504          ...          ...           ...           ...
31505          ...          ...           ...           ...
31506          ...          ...           ...           ...

      Fwd Packet Length Mean  Fwd IAT Std  Packet Length Mean \

```

0	19.833334	98776.15	322.16666
1	0.000000	0.00	0.00000
2	6.000000	0.00	6.00000
3	36.000000	0.00	42.40000
4	6.000000	0.00	6.00000
...
31502	0.000000	4037277.80	0.00000
31503	0.000000	4144374.80	0.00000
31504	0.000000	4139029.80	0.00000
31505	0.000000	3927356.50	0.00000
31506	0.000000	3547404.80	0.00000

	Fwd Packet Length	Max	Subflow Fwd Packets	Flow Packets/s	\
0	119		6	36.258636	
1	0		1	17094.018000	
2	6		2	14084.507000	
3	36		2	20942.408000	
4	6		2	500000.000000	
...
31502	0		3	0.700408	
31503	0		3	0.682296	
31504	0		3	0.683192	
31505	0		3	0.720001	
31506	0		3	0.797098	

	Total Fwd Packets	Destination Port	Label
0	6	443	Benign
1	1	52631	Benign
2	2	80	Benign
3	2	53	Benign
4	2	49467	Benign
...
31502	3	80	Brute Force
31503	3	80	Brute Force
31504	3	80	Brute Force
31505	3	80	Brute Force
31506	3	80	Brute Force

[31507 rows x 17 columns]

```
[8]: def plot_class_distribution(
    df,
    name_fig='class_distribution',
    label_col='Label',
    save_path='./plots/',
    fig_size=(8, 5),
    palette='pastel'
```

```

):
"""
Plot the number of samples for each class.

Args:
    df (pd.DataFrame): The input DataFrame.
    label_col (str): The name of the label column. Defaults to 'Label'.
    save_path (str): The directory to save the plot. Defaults to './plots/'.
    fig_size (tuple): Size of the figure. Defaults to (8, 5).
    palette (str): Seaborn palette.

"""
os.makedirs(save_path, exist_ok=True)

# Create a figure and axes for the plot
fig, ax = plt.subplots(figsize=fig_size)

# Create a countplot showing the distribution of classes
sns.countplot(x=label_col, data=df, order=df[label_col].value_counts() .
index, ax=ax, palette=palette, hue=label_col, legend=False)

# Set the title and labels for the plot
ax.set_title("Class Distribution")
ax.set_xlabel("Traffic Type")
ax.set_ylabel("Count")

# Rotate x-axis labels for better readability
plt.xticks(rotation=30)

# Annotate bars with counts
for p in ax.patches:
    height = p.get_height()
    ax.annotate(f'{height}', (p.get_x() + p.get_width() / 2., height),
                ha='center', va='bottom', fontsize=10)

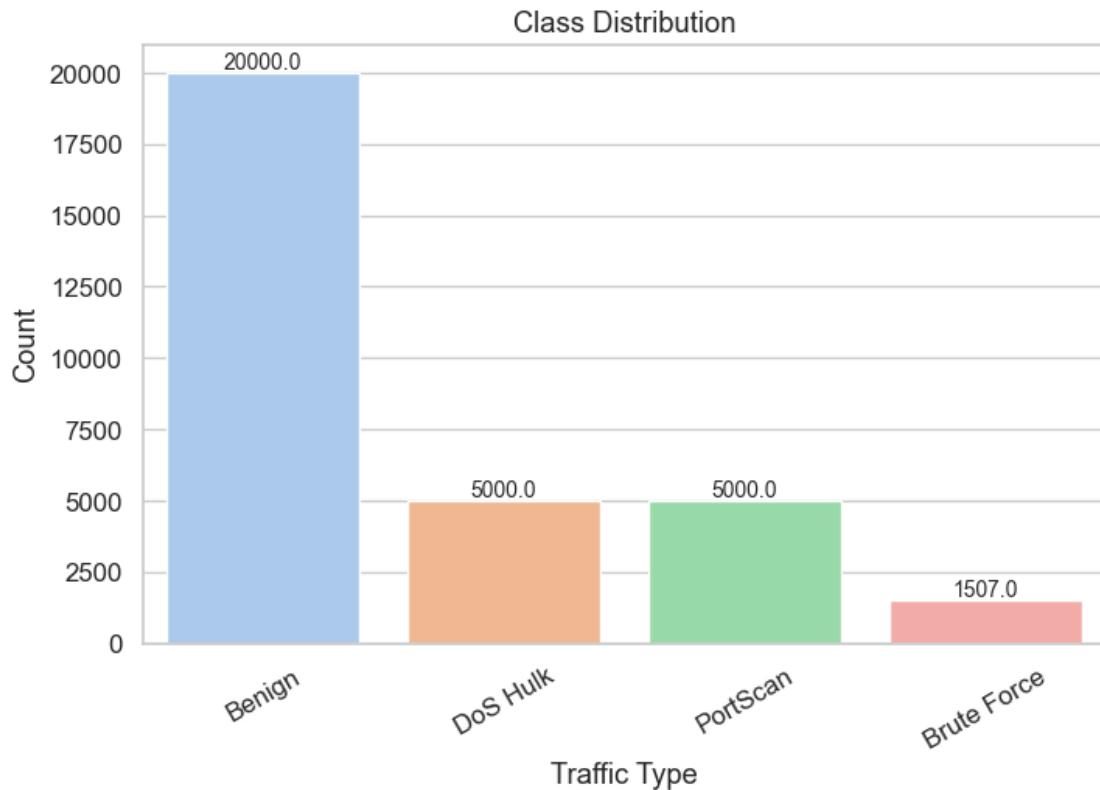
# Save the plot to the specified path
save_plot(fig, name_fig, save_path)

```

[9]: # --- Visualize raw data characteristics and distributions ---

```
# Plot class distribution to understand data balance
plot_class_distribution(df, 'class_distribution', save_path=save_dir)
```

Saved plot: ../results/images/task1_plots/class_distribution.png



1.2.1 Removing NaN and duplicates

```
[10]: # --- Remove NaN and duplicates ---

raw_n = len(df)

# Drop NaN
df = df.dropna()
clean_n = len(df)
print(f"Removed {raw_n-clean_n} rows (NaN)")

# Drop duplicates
df = df.drop_duplicates()
clean_n = len(df)
print(f"Removed {raw_n-clean_n} rows (duplicates)")

print(f"New shape: {df.shape}")
```

Removed 20 rows (NaN)
 Removed 2114 rows (duplicates)
 New shape: (29393, 17)

```
[11]: # --- Handle infinite values ---

# Replace infinite values with NaN
df.replace([np.inf, -np.inf], np.nan, inplace=True)

# Check for and report the number of infinite values (now NaNs)
inf_counts = df.isnull().sum()
print("\nNumber of infinite values (replaced with NaN) per column:")
print(inf_counts[inf_counts > 0])

# Drop rows with NaN values (including those that were originally infinite)
initial_rows = len(df)
df.dropna(inplace=True)
rows_after_inf_nan_drop = len(df)

print(f"\nRemoved {initial_rows - rows_after_inf_nan_drop} rows containing"
      " infinite or NaN values. New shape: {df.shape}")
```

Number of infinite values (replaced with NaN) per column:
Flow Bytes/s 7
Flow Packets/s 7
dtype: int64

Removed 7 rows containing infinite or NaN values. New shape: (29386, 17)

Q: How many samples did you have before and after removing missing and duplicates entries? We initially had **31507** samples bold text, and after removing missing, duplicate, and infinite entries, we obtained 29,386 clean samples. In total, **2121** (2114 missing and duplicates + 7 infinite values) rows **were removed** during the data cleaning process.

```
[12]: print("\nLabel distribution (after NaN and duplicates removal):")
print(df['Label'].value_counts())
```

Label distribution (after NaN and duplicates removal):
Label
Benign 19242
PortScan 4849
DoS Hulk 3868
Brute Force 1427
Name: count, dtype: int64

```
[13]: # Encode labels
label_encoder = LabelEncoder()
df['Label'] = label_encoder.fit_transform(df['Label'])

df.head(10)
```

[13]:	Flow Duration	Flow IAT Mean	Fwd PSH Flags	Bwd Packet Length Mean	\
0	303376	3.033760e+04	0	749.400000	
1	117	1.170000e+02	0	0.000000	
2	142	1.420000e+02	0	0.000000	
3	191	6.366667e+01	0	52.000000	
4	4	4.000000e+00	0	0.000000	
5	162322	3.959073e+03	0	19.416666	
6	61050653	2.907174e+06	0	22.818182	
7	108	1.080000e+02	0	0.000000	
8	764920	7.649200e+05	0	0.000000	
9	122255	6.112750e+04	0	0.000000	
	Bwd Packet Length Max	Flow Bytes/s	Down/Up Ratio	SYN Flag Count	\
0	1448	1.274326e+04	0	0	
1	0	0.000000e+00	1	0	
2	0	8.450704e+04	0	0	
3	52	9.214659e+05	1	0	
4	0	3.000000e+06	0	0	
5	51	4.102956e+03	1	0	
6	233	5.230083e+01	1	0	
7	0	1.111111e+05	0	0	
8	0	1.568792e+01	0	0	
9	0	0.000000e+00	0	0	
	Fwd Packet Length Mean	Fwd IAT Std	Packet Length Mean	\	
0	19.833334	98776.150	322.166660		
1	0.000000	0.000	0.000000		
2	6.000000	0.000	6.000000		
3	36.000000	0.000	42.400000		
4	6.000000	0.000	6.000000		
5	11.111111	30630.129	15.488372		
6	267.454560	5145240.000	138.826080		
7	6.000000	0.000	6.000000		
8	6.000000	0.000	6.000000		
9	0.000000	0.000	0.000000		
	Fwd Packet Length Max	Subflow Fwd Packets	Flow Packets/s	\	
0	119	6	36.258636		
1	0	1	17094.018000		
2	6	2	14084.507000		
3	36	2	20942.408000		
4	6	2	500000.000000		
5	43	18	258.744960		
6	1460	11	0.360357		
7	6	2	18518.518000		
8	6	2	2.614652		
9	0	2	24.538874		

	Total Fwd Packets	Destination Port	Label
0	6	443	0
1	1	52631	0
2	2	80	0
3	2	53	0
4	2	49467	0
5	18	21	0
6	11	80	0
7	2	80	0
8	2	443	0
9	2	443	0

```
[14]: # --- Display the label encoding mapping ---
print("\nLabel Encoding Mapping:")
for i, label in enumerate(label_encoder.classes_):
    print(f"[label]: {i}")
```

Label Encoding Mapping:

Benign: 0
Brute Force: 1
DoS Hulk: 2
PortScan: 3

```
[15]: # Checking again null values
print(df.isnull().sum())
```

Flow Duration	0
Flow IAT Mean	0
Fwd PSH Flags	0
Bwd Packet Length Mean	0
Bwd Packet Length Max	0
Flow Bytes/s	0
Down/Up Ratio	0
SYN Flag Count	0
Fwd Packet Length Mean	0
Fwd IAT Std	0
Packet Length Mean	0
Fwd Packet Length Max	0
Subflow Fwd Packets	0
Flow Packets/s	0
Total Fwd Packets	0
Destination Port	0
Label	0

dtype: int64

```
[16]: # Checking again for the infinite values
print(df.isin([np.inf, -np.inf]).sum())
```

```
Flow Duration      0
Flow IAT Mean     0
Fwd PSH Flags     0
Bwd Packet Length Mean 0
Bwd Packet Length Max 0
Flow Bytes/s      0
Down/Up Ratio     0
SYN Flag Count    0
Fwd Packet Length Mean 0
Fwd IAT Std       0
Packet Length Mean 0
Fwd Packet Length Max 0
Subflow Fwd Packets 0
Flow Packets/s    0
Total Fwd Packets 0
Destination Port   0
Label              0
dtype: int64
```

1.2.2 Split data

We use a **stratified approach** due to the class imbalance.

```
[17]: # --- Split data ---

# Split features/target
label_col = 'Label'
feature_cols = [c for c in df.columns if c != label_col]
X = df[feature_cols].values
y = df[label_col].values

# Train/val/test split 60/20/20 with stratify
X_train, X_tmp, y_train, y_tmp = train_test_split(
    X, y, test_size=0.4, stratify=y, random_state=42
)
X_val, X_test, y_val, y_test = train_test_split(
    X_tmp, y_tmp, test_size=0.5, stratify=y_tmp, random_state=42
)

print("Data Splits:")
print(f"Train set: {X_train.shape[0]} samples")
print(f"Validation set: {X_val.shape[0]} samples")
print(f"Test set: {X_test.shape[0]} samples\n")

def print_label_counts(name, y):
```

```

labels, counts = np.unique(y, return_counts=True)
count_width = 6
print(f"{'name':<8}", end=" ")
for label, count in zip(labels, counts):
    print(f"{'label':>{count_width},}", end="   ")
print()

print_label_counts("Train", y_train)
print_label_counts("Val", y_val)
print_label_counts("Test", y_test)

```

Data Splits:

Train set: 17,631 samples
Validation set: 5,877 samples
Test set: 5,878 samples

Train	0: 11,545	1: 856	2: 2,321	3: 2,909
Val	0: 3,848	1: 286	2: 773	3: 970
Test	0: 3,849	1: 285	2: 774	3: 970

1.2.3 Outliers Detection

```
[18]: # --- Outlier detection (Z-score and IQR) ---

# Convert X_train to DataFrame to use select_dtypes
X_train_df = pd.DataFrame(X_train, columns=feature_cols)

num_cols = X_train_df.select_dtypes(include=[np.number]).columns.tolist()
print(num_cols)

# Z-score method
zs = ((X_train_df[num_cols] - X_train_df[num_cols].mean()) / 
      X_train_df[num_cols].std(ddof=0)).abs()
outlier_counts_z = (zs > 3).sum().sort_values(ascending=False)
print("\n[Z-SCORE OUTLIERS] features:")
print(outlier_counts_z)

# IQR method
Q1 = X_train_df[num_cols].quantile(0.25)
Q3 = X_train_df[num_cols].quantile(0.75)
IQR = Q3 - Q1
outliers_iqr = ((X_train_df[num_cols] < (Q1 - 1.5 * IQR)) | 
                  (X_train_df[num_cols] > (Q3 + 1.5 * IQR))).sum()
outlier_counts_iqr = outliers_iqr.sort_values(ascending=False)
print("\n[IQR OUTLIERS] features:")
print(outlier_counts_iqr)
```

['Flow Duration', 'Flow IAT Mean', 'Fwd PSH Flags', 'Bwd Packet Length Mean',

```
'Bwd Packet Length Max', 'Flow Bytes/s', 'Down/Up Ratio', 'SYN Flag Count', 'Fwd Packet Length Mean', 'Fwd IAT Std', 'Packet Length Mean', 'Fwd Packet Length Max', 'Subflow Fwd Packets', 'Flow Packets/s', 'Total Fwd Packets', 'Destination Port']
```

[Z-SCORE OUTLIERS] features:

```
Fwd PSH Flags      708  
SYN Flag Count    708  
Fwd IAT Std       567  
Bwd Packet Length Max 523  
Flow Packets/s    522  
Bwd Packet Length Mean 340  
Packet Length Mean 272  
Destination Port   247  
Fwd Packet Length Max 238  
Flow IAT Mean      207  
Fwd Packet Length Mean 157  
Subflow Fwd Packets 88  
Total Fwd Packets  88  
Down/Up Ratio      48  
Flow Bytes/s       37  
Flow Duration       0  
dtype: int64
```

[IQR OUTLIERS] features:

```
Bwd Packet Length Max 3951  
Destination Port      3879  
Flow Duration         3443  
Bwd Packet Length Mean 3180  
Packet Length Mean    2982  
Flow IAT Mean          2913  
Flow Bytes/s           2826  
Fwd IAT Std            2662  
Subflow Fwd Packets   1467  
Total Fwd Packets     1467  
Flow Packets/s         1417  
Fwd Packet Length Mean 997  
Fwd Packet Length Max  929  
Fwd PSH Flags          708  
SYN Flag Count         708  
Down/Up Ratio          48  
dtype: int64
```

```
[19]: # --- Visualize raw distributions for selected features ---
```

```
selected_features = [  
    'Flow Duration', 'Flow IAT Mean', 'Bwd Packet Length Mean',
```

```

'Bwd Packet Length Max', 'Flow Bytes/s', 'Fwd Packet Length Mean',
'Fwd IAT Std', 'Packet Length Mean', 'Fwd Packet Length Max', 'Flow Packets/
↳S'
]

# Convert X_train to DataFrame for easier plotting with column names
X_train_df = pd.DataFrame(X_train, columns=feature_cols)

def plot_distributions(df, features, title_prefix, save_name):
    n = len(features)
    fig, axes = plt.subplots(nrows=n, ncols=2, figsize=(10, 3 * n))

    for i, col in enumerate(features):
        # KDE Plot
        sns.kdeplot(df[col], ax=axes[i, 0], fill=True, color="steelblue")
        axes[i, 0].set_title(f"{title_prefix} - KDE: {col}")
        axes[i, 0].set_xlabel("")

        # Boxplot
        sns.boxplot(x=df[col], ax=axes[i, 1], color="lightcoral")
        axes[i, 1].set_title(f"{title_prefix} - Boxplot: {col}")
        axes[i, 1].set_xlabel("")

    plt.tight_layout()

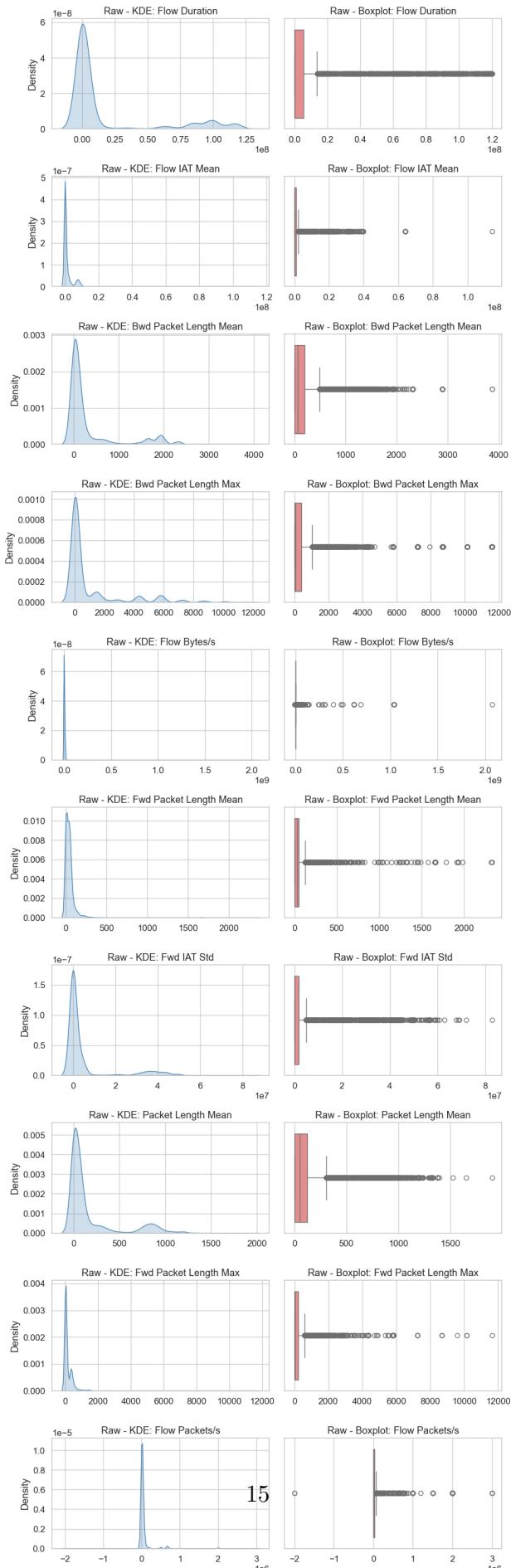
# Save the plot to the specified path
save_plot(fig, save_name, save_dir, fmt='pdf')

plt.show()

plot_distributions(X_train_df, selected_features, "Raw", "raw_distributions")

```

Saved plot: ../results/images/task1_plots/raw_distributions.pdf



1.2.4 Data Normalization

```
[20]: # Standardize the features (StandardScaler)
scaler1 = StandardScaler()
X_train_std = scaler1.fit_transform(X_train)
X_val_std = scaler1.transform(X_val)
X_test_std = scaler1.transform(X_test)

# Standardize the features (RobustScaler)
scaler2 = RobustScaler()
X_train_rob = scaler2.fit_transform(X_train)
X_val_rob = scaler2.transform(X_val)
X_test_rob = scaler2.transform(X_test)
```

```
[21]: # --- Visual comparison of Standard vs Robust scaling ---

# Convert scaled arrays back to DataFrames for easier plotting with column names
X_train_std_df = pd.DataFrame(X_train_std, columns=feature_cols)
X_train_rob_df = pd.DataFrame(X_train_rob, columns=feature_cols)

# Adjust subplot grid to accommodate all selected features (10 features, 5 rows
# x 2 columns)
fig, axes = plt.subplots(5, 2, figsize=(10, 20)) # Increased figsize for better
# readability

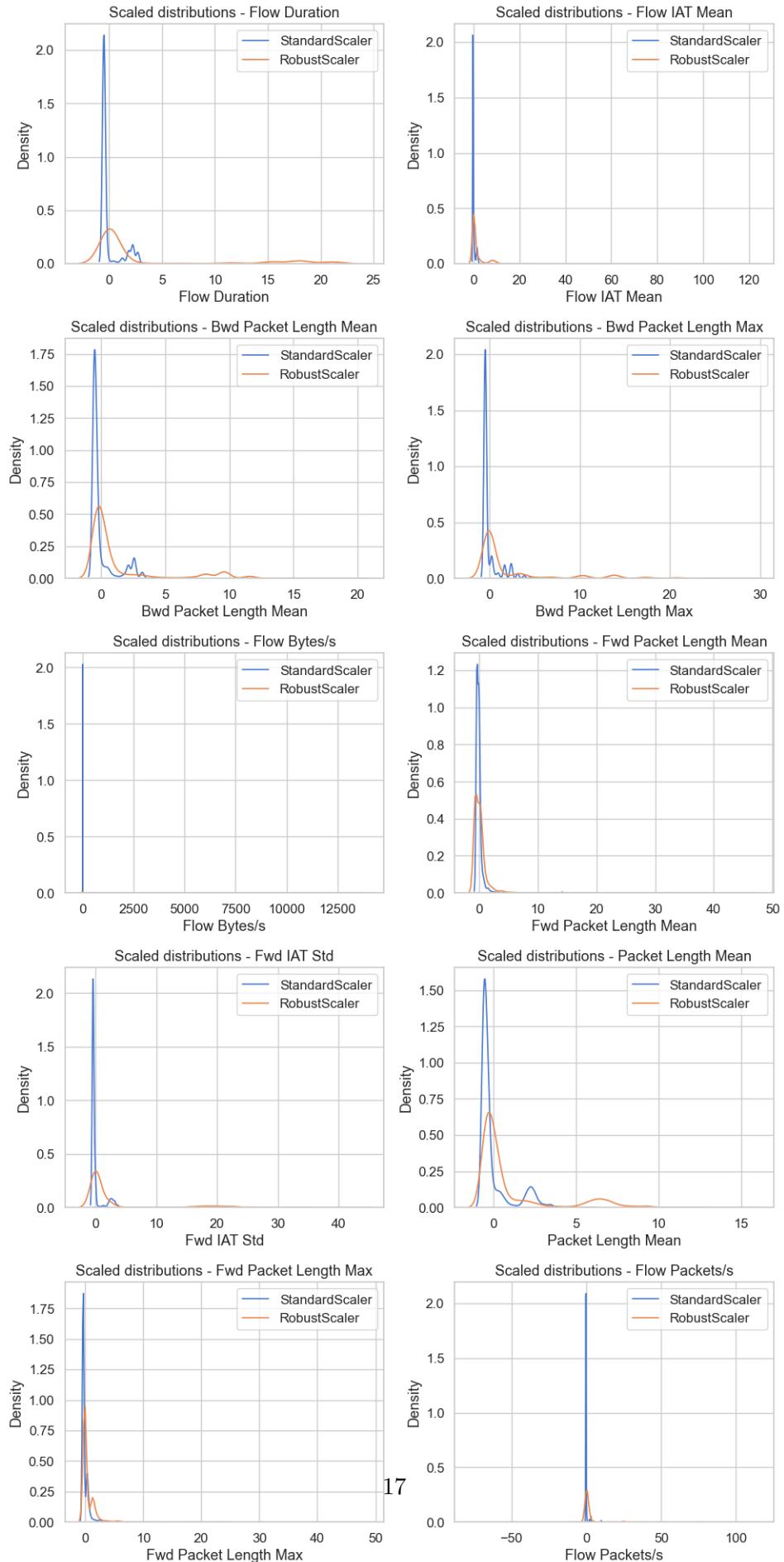
# Plot all selected features for comparison
for i, col in enumerate(selected_features):
    row_idx = i // 2
    col_idx = i % 2
    sns.kdeplot(X_train_std_df[col], ax=axes[row_idx, col_idx], color="blue",
                 label="StandardScaler", lw=1.2)
    sns.kdeplot(X_train_rob_df[col], ax=axes[row_idx, col_idx], color="red",
                 label="RobustScaler", lw=1.2)
    axes[row_idx, col_idx].set_title(f"Scaled distributions - {col}")
    axes[row_idx, col_idx].legend()

plt.tight_layout()

# Save the plot to the specified path
save_plot(fig, 'raw_distributions_comparison', save_dir, fmt='pdf')

plt.show()
plt.close(fig)
```

Saved plot: ../results/images/task1_plots/raw_distributions_comparison.pdf



```
[22]: # --- Compare scaling statistics numerically ---

stats_std = X_train_std_df.describe().T[['mean', 'std']].rename(columns={'mean':
    ↵ 'mean_std', 'std': 'std_std'})
stats_rob = X_train_rob_df.describe().T[['mean', 'std']].rename(columns={'mean':
    ↵ 'mean_rob', 'std': 'std_rob'})
scaling_comparison = stats_std.join(stats_rob)

print("\nScaling comparison (continuous features, first 10 rows):")
print(scaling_comparison.head(10))
```

Scaling comparison (continuous features, first 10 rows):

	mean_std	std_std	mean_rob	std_rob
Flow Duration	-1.612030e-18	1.000028	3.209521	6.578692
Flow IAT Mean	4.693024e-16	1.000028	1.655390	4.604932
Fwd PSH Flags	1.652331e-17	1.000028	0.040157	0.196332
Bwd Packet Length Mean	-7.245271e-15	1.000028	1.366380	3.176369
Bwd Packet Length Max	2.579249e-17	1.000028	2.137739	4.824989
Flow Bytes/s	7.818348e-17	1.000028	10.549447	192.030725
Down/Up Ratio	5.642107e-17	1.000028	-0.333503	0.523037
SYN Flag Count	1.652331e-17	1.000028	0.040157	0.196332
Fwd Packet Length Mean	1.018803e-15	1.000028	0.251230	2.318150
Fwd IAT Std	-2.954046e-16	1.000028	2.570055	6.266235

Q: How did you normalize the data? Why did you choose it? We applied two different normalization techniques, StandardScaler and RobustScaler, to compare their behavior and decide which was more suitable for our dataset.

- **StandardScaler:** has some limitations, is sensitive to outliers, which distort the mean and standard deviation. Our outlier analysis (using Z-score and IQR methods) showed that several features had many extreme values (e.g. Bwd Packet Length Max, Flow Duration, Bwd Packet Length Mean, and Fwd IAT Std had thousands of outliers).
- **RobustScaler:** This approach is less sensitive to outliers, as it relies on statistics (median and IQR) that are not affected by extreme values. In the comparison plots, the scaled distributions were more compact and less skewed, especially for features with strong outliers like Bwd Packet Length Max, Flow Duration, Bwd Packet Length Mean, and Fwd IAT Std. However, the mean and standard deviation varied across features, which is expected since RobustScaler does not enforce a standard normal distribution.

Despite RobustScaler being more robust to extreme values, we ultimately chose **StandardScaler** for our dataset. The comparison plots showed that the loss curves during training were smoother using the standard standardization, and the performance of preliminary models was very similar between the two scalers. Using StandardScaler also simplifies interpretation.

1.3 Task 2 — Shallow Neural Network (1 layer)

We design and train three shallow FFNN models with a single hidden layer, varying the hidden size.

Configuration: - Hidden layer sizes: **{32, 64, 128}** - Activation: **Linear** (first run) - Optimizer: **AdamW**, learning rate = 5e-4 - Batch size: **64** - Loss function: **CrossEntropyLoss** - Early stopping up to **100 epochs**

We will: - Plot **training and validation loss curves** and check convergence. - Select the best model based on validation loss. - Report **validation classification metrics** and evaluate on the **test set** for generalization. - Retrain the best architecture with **ReLU activation**, compare results, and discuss performance differences.

```
[23]: # Create directory for plots
save_dir = results_path + 'images/' + 'task2_plots/'
os.makedirs(save_dir, exist_ok=True)
```

1.3.1 Training

```
[24]: # --- Choose dataset version and create DataLoaders ---
X_train_use = X_train_std # change here if you want RobustScaler
X_val_use   = X_val_std
X_test_use  = X_test_std

# Convert to PyTorch tensors
X_train_tensor = torch.tensor(X_train_use, dtype=torch.float32)
X_val_tensor   = torch.tensor(X_val_use, dtype=torch.float32)
X_test_tensor  = torch.tensor(X_test_use, dtype=torch.float32)

y_train_tensor = torch.tensor(y_train, dtype=torch.long)
y_val_tensor   = torch.tensor(y_val, dtype=torch.long)
y_test_tensor  = torch.tensor(y_test, dtype=torch.long)

# Create DataLoaders
batch_size     = 64
train_loader   = DataLoader(TensorDataset(X_train_tensor, y_train_tensor), □
    ↪batch_size=batch_size, shuffle=True)
val_loader     = DataLoader(TensorDataset(X_val_tensor, y_val_tensor), □
    ↪batch_size=batch_size, shuffle=False)
```

```
[25]: # --- Define single-layer NN class ---
class ShallowNN(nn.Module):
    def __init__(self, input_dim, hidden_dim, output_dim, activation='linear'):
        super(ShallowNN, self).__init__()
        self.fc = nn.Linear(input_dim, hidden_dim)
        self.out = nn.Linear(hidden_dim, output_dim)
```

```

    if activation == 'relu':
        self.activation = nn.ReLU()
    elif activation == 'linear':
        self.activation = nn.Identity()
    else:
        raise ValueError("Invalid activation function. Use 'relu' or"
                         "'linear'.")

```

```

def forward(self, x):
    x = self.fc(x)
    x = self.activation(x)
    return self.out(x)

```

[26]: # --- Training function with early stopping ---

```

def train_model(model, train_loader, val_loader, epochs, optimizer, criterion,
                min_delta=None, patience=None):

    train_losses, val_losses = [], []
    best_val_loss = float('inf')
    best_model_state = None
    counter = 0

    for epoch in range(epochs):
        # Training
        model.train()
        batch_losses = []
        for X_batch, y_batch in train_loader:
            optimizer.zero_grad()
            outputs = model(X_batch)
            loss = criterion(outputs, y_batch)
            loss.backward()
            optimizer.step()
            batch_losses.append(loss.item())
        train_loss = np.mean(batch_losses)

        # Validation
        model.eval()
        val_batch_losses = []
        with torch.no_grad():
            for X_batch, y_batch in val_loader:
                outputs = model(X_batch)
                loss = criterion(outputs, y_batch)
                val_batch_losses.append(loss.item())
        val_loss = np.mean(val_batch_losses)

        train_losses.append(train_loss)

```

```

    val_losses.append(val_loss)

    # Early Stopping
    if(min_delta!= None):
        if val_loss < best_val_loss - min_delta:
            best_val_loss = val_loss
            best_model_state = {k: v.cpu().clone() for k, v in model.
        ↪state_dict().items()}
            trigger_times = 0
        else:
            trigger_times += 1
            if trigger_times >= patience:
                print(f"Early stopping at epoch {epoch+1} (best val loss: {best_val_loss:.6f})")
                break

    # Restore best model
    if best_model_state is not None:
        model.load_state_dict(best_model_state)

    if (epoch+1) % 5 == 0 or epoch == 0 or epoch == epochs:
        print(f"Epoch {epoch+1}/{epochs} - Train Loss: {train_loss:.4f},"
        ↪Val Loss: {val_loss:.4f}")

    # Load best weights
    model.load_state_dict(best_model_state)
    return model, train_losses, val_losses

```

[27]: # --- Train the three models with different neurons (Linear activation) ---

```

input_dim = X_train_use.shape[1]
output_dim = len(np.unique(y_train))
neurons_list = [32, 64, 128]

trained_models = {}
loss_curves = {}

# Initialize the early stopping parameters
min_delta_dict = {32: 0.00001, 64: 0.00001, 128: 0.00001}
patience_dict = {32: 20, 64: 20, 128: 20}
# It is possible to try also other values, but these work fine (same as
↪professor's)

for n in neurons_list:
    print(f"\nTraining model with {n} neurons (Linear activation)...")

    # Set hyperparameters

```

```

model = ShallowNN(input_dim, n, output_dim, activation='linear')
criterion = nn.CrossEntropyLoss()
optimizer = optim.AdamW(model.parameters(), lr=0.0005)
epochs = 100

# Move model to device
model = model.to(device)

# Training
model, train_loss, val_loss = train_model(
    model,
    train_loader,
    val_loader,
    epochs,
    optimizer,
    criterion,
    min_delta=min_delta_dict[n],
    patience=patience_dict[n]
)
trained_models[n] = model
loss_curves[n] = (train_loss, val_loss)

```

Training model with 32 neurons (Linear activation)...

Epoch 1/100 - Train Loss: 0.9124, Val Loss: 0.6639
 Epoch 5/100 - Train Loss: 0.4107, Val Loss: 0.3888
 Epoch 10/100 - Train Loss: 0.3599, Val Loss: 0.3483
 Epoch 15/100 - Train Loss: 0.3428, Val Loss: 0.3316
 Epoch 20/100 - Train Loss: 0.3321, Val Loss: 0.3210
 Epoch 25/100 - Train Loss: 0.3268, Val Loss: 0.3153
 Epoch 30/100 - Train Loss: 0.3242, Val Loss: 0.3127
 Epoch 35/100 - Train Loss: 0.3212, Val Loss: 0.3105
 Epoch 40/100 - Train Loss: 0.3167, Val Loss: 0.3058
 Epoch 45/100 - Train Loss: 0.3149, Val Loss: 0.3040
 Epoch 50/100 - Train Loss: 0.3125, Val Loss: 0.3021
 Epoch 55/100 - Train Loss: 0.3118, Val Loss: 0.3027
 Epoch 60/100 - Train Loss: 0.3114, Val Loss: 0.3018
 Epoch 65/100 - Train Loss: 0.3107, Val Loss: 0.3028
 Epoch 70/100 - Train Loss: 0.3105, Val Loss: 0.3024
 Epoch 75/100 - Train Loss: 0.3092, Val Loss: 0.3004
 Epoch 80/100 - Train Loss: 0.3083, Val Loss: 0.2991
 Epoch 85/100 - Train Loss: 0.3071, Val Loss: 0.3002
 Epoch 90/100 - Train Loss: 0.3069, Val Loss: 0.2995
 Epoch 95/100 - Train Loss: 0.3061, Val Loss: 0.2988
 Epoch 100/100 - Train Loss: 0.3045, Val Loss: 0.2951

Training model with 64 neurons (Linear activation)...

Epoch 1/100 - Train Loss: 0.7937, Val Loss: 0.5589

```
Epoch 5/100 - Train Loss: 0.3871, Val Loss: 0.3687
Epoch 10/100 - Train Loss: 0.3508, Val Loss: 0.3363
Epoch 15/100 - Train Loss: 0.3344, Val Loss: 0.3230
Epoch 20/100 - Train Loss: 0.3277, Val Loss: 0.3172
Epoch 25/100 - Train Loss: 0.3236, Val Loss: 0.3104
Epoch 30/100 - Train Loss: 0.3193, Val Loss: 0.3073
Epoch 35/100 - Train Loss: 0.3184, Val Loss: 0.3048
Epoch 40/100 - Train Loss: 0.3165, Val Loss: 0.3034
Epoch 45/100 - Train Loss: 0.3149, Val Loss: 0.3020
Epoch 50/100 - Train Loss: 0.3132, Val Loss: 0.3059
Epoch 55/100 - Train Loss: 0.3118, Val Loss: 0.3009
Epoch 60/100 - Train Loss: 0.3109, Val Loss: 0.3010
Epoch 65/100 - Train Loss: 0.3085, Val Loss: 0.2964
Epoch 70/100 - Train Loss: 0.3076, Val Loss: 0.2966
Epoch 75/100 - Train Loss: 0.3066, Val Loss: 0.2973
Epoch 80/100 - Train Loss: 0.3078, Val Loss: 0.2958
Epoch 85/100 - Train Loss: 0.3087, Val Loss: 0.2969
Early stopping at epoch 88 (best val loss: 0.295718)
```

```
Training model with 128 neurons (Linear activation)...
Epoch 1/100 - Train Loss: 0.7008, Val Loss: 0.4888
Epoch 5/100 - Train Loss: 0.3686, Val Loss: 0.3516
Epoch 10/100 - Train Loss: 0.3422, Val Loss: 0.3282
Epoch 15/100 - Train Loss: 0.3322, Val Loss: 0.3197
Epoch 20/100 - Train Loss: 0.3261, Val Loss: 0.3105
Epoch 25/100 - Train Loss: 0.3227, Val Loss: 0.3078
Epoch 30/100 - Train Loss: 0.3179, Val Loss: 0.3024
Epoch 35/100 - Train Loss: 0.3174, Val Loss: 0.3031
Epoch 40/100 - Train Loss: 0.3167, Val Loss: 0.3015
Epoch 45/100 - Train Loss: 0.3157, Val Loss: 0.3028
Epoch 50/100 - Train Loss: 0.3153, Val Loss: 0.3045
Epoch 55/100 - Train Loss: 0.3151, Val Loss: 0.3004
Epoch 60/100 - Train Loss: 0.3115, Val Loss: 0.2988
Epoch 65/100 - Train Loss: 0.3108, Val Loss: 0.2981
Epoch 70/100 - Train Loss: 0.3094, Val Loss: 0.2967
Epoch 75/100 - Train Loss: 0.3075, Val Loss: 0.2958
Epoch 80/100 - Train Loss: 0.3072, Val Loss: 0.3014
Epoch 85/100 - Train Loss: 0.3028, Val Loss: 0.2935
Epoch 90/100 - Train Loss: 0.3059, Val Loss: 0.2942
Epoch 95/100 - Train Loss: 0.3028, Val Loss: 0.2977
Epoch 100/100 - Train Loss: 0.3040, Val Loss: 0.2974
```

1.3.2 Evaluation

```
[28]: # --- Plot loss curves for all models ---

for n in neurons_list:
```

```

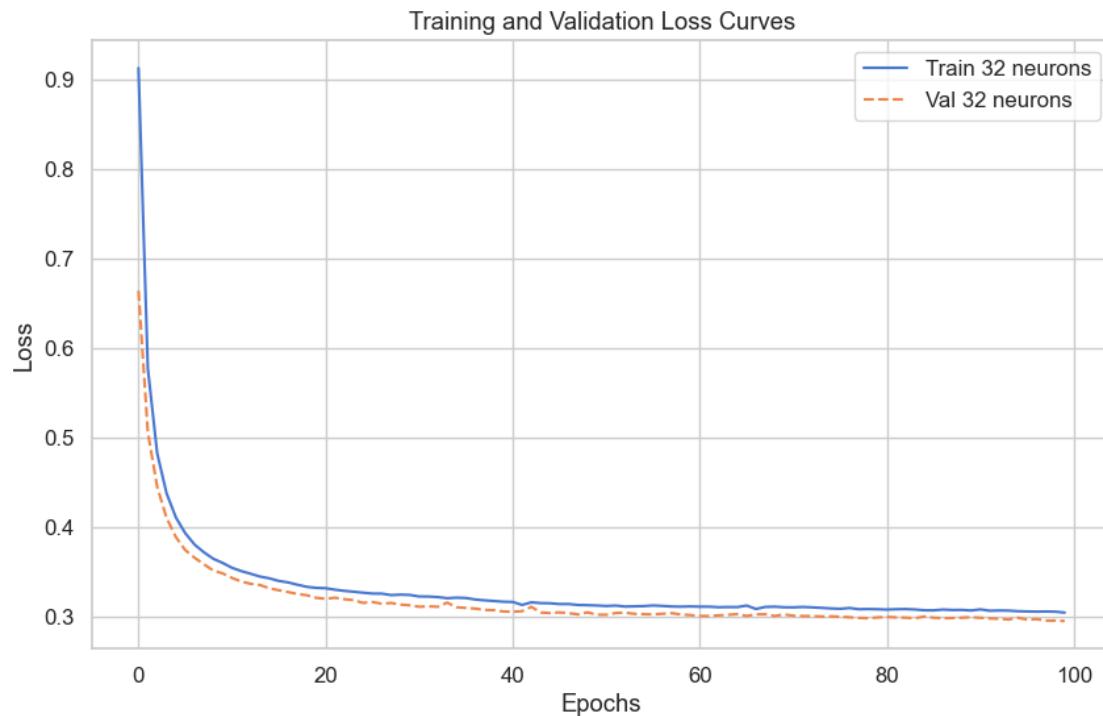
plt.figure(figsize=(10,6))
train_loss, val_loss = loss_curves[n]
plt.plot(train_loss, label=f'Train {n} neurons')
plt.plot(val_loss, '--', label=f'Val {n} neurons')
plt.xlabel('Epochs')
plt.ylabel('Loss')
plt.title('Training and Validation Loss Curves')
plt.legend()

# Save the plot to the specified path
save_plot(plt.gcf(), f"loss_curves_model_{n}", save_dir)

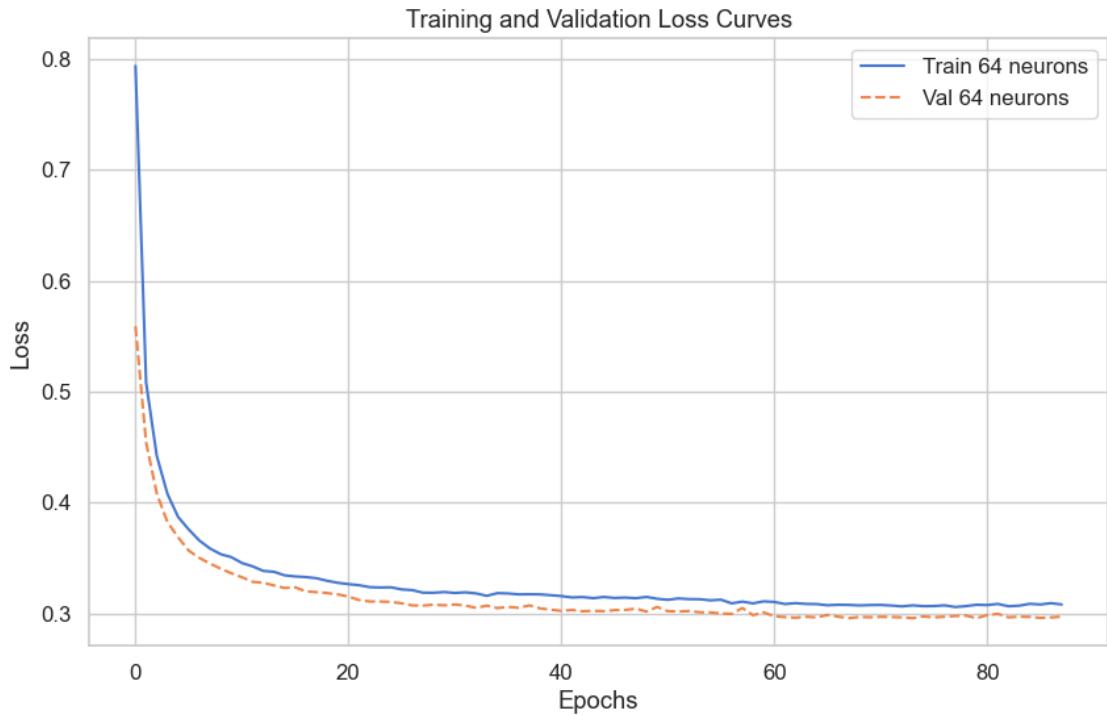
plt.show()

```

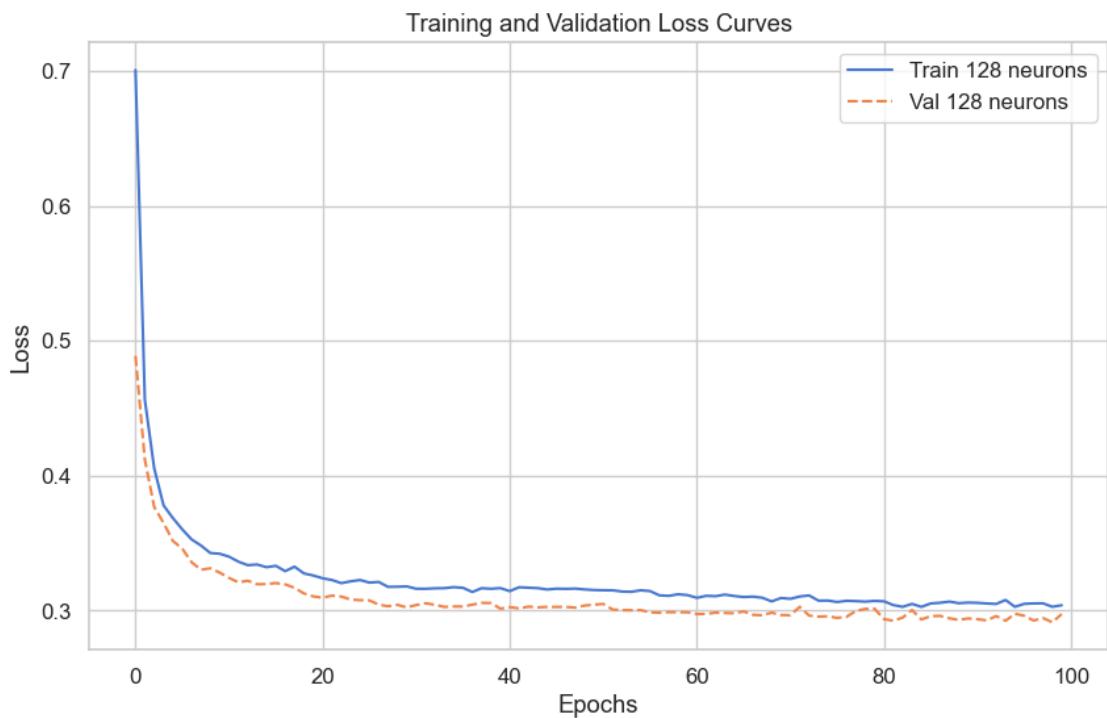
Saved plot: ../results/images/task2_plots/loss_curves_model_32.png



Saved plot: ../results/images/task2_plots/loss_curves_model_64.png



Saved plot: ./results/images/task2_plots/loss_curves_model_128.png



Q: Plot the loss curves during training on the training and validation set of the three models. What is their evolution? Do they converge? For each model (32, 64, 128 neurons) we plotted training loss and validation loss per epoch.

We would like to specify that these values refer to a specific run. They might change if the notebook is processed again.

32 neurons:

- Training loss: started ~ 0.91 (epoch 1) and decreased steadily to ~ 0.30 by epoch 100.
- Validation loss: started ~ 0.66 and decreased to ~ 0.29 by the end.

64 neurons:

- Training loss: started $\sim 0.79 \rightarrow \sim 0.30$ when training stopped.
- Validation loss: started $\sim 0.55 \rightarrow \sim 0.29$. Early stopping triggered at epoch 78 (best val loss 0.295).

128 neurons:

- Training loss: started ~ 0.70 and hovered around ~ 0.30 at epoch 100.
- Validation loss: started ~ 0.48 and reached ~ 0.29 as best value.

All three models show clear convergence behavior:

- Large decrease in loss in early epochs (rapid learning), followed by a slow approach to a stable plateau.
- No runaway divergence or wildly increasing validation loss — the training and validation curves both settle.

Q: How do you select the best model across epochs? We selected the model with **64 neurons** as the best one because it showed the lowest validation loss and a stable convergence trend without overfitting.

```
[36]: def evaluate_model(model, X_tensor, y_true, model_name: str = "Unnamed model"):  
    """  
        Evaluate a trained model on a given dataset and return the classification report.  
  
        Handles missing predicted classes gracefully (zero_division=0) and reports which classes were not predicted, along with the model/config name.  
    """  
  
    model.eval()  
    with torch.no_grad():  
        outputs = model(X_tensor)  
        y_pred = torch.argmax(outputs, dim=1).cpu().numpy()  
  
        # Convert y_true to numpy if it's a tensor  
        if isinstance(y_true, torch.Tensor):  
            y_true = y_true.cpu().numpy()
```

```

# Identify missing classes (not predicted at all)
missing_classes = set(np.unique(y_true)) - set(np.unique(y_pred))
if missing_classes:
    # Convert NumPy types to plain ints for readability
    missing_classes = [int(x) for x in sorted(missing_classes)]
    print(f"Warning: {model_name} made no predictions for classes: {missing_classes}")

# Generate classification report without raising warnings
report = classification_report(y_true, y_pred, digits=4, zero_division=0)

return report

```

[37]: # --- Evaluate validation set and print classification reports ---

```

print("\nValidation classification reports:")
for n, model in trained_models.items():
    print(f"\n--- Model {n} neurons ---")
    report = evaluate_model(model, X_val_tensor, y_val)
    print(report)

```

Validation classification reports:

--- Model 32 neurons ---

	precision	recall	f1-score	support
0	0.8855	0.9545	0.9187	3848
1	0.0000	0.0000	0.0000	286
2	0.9883	0.8758	0.9287	773
3	0.8343	0.8876	0.8601	970
accuracy			0.8867	5877
macro avg	0.6770	0.6795	0.6769	5877
weighted avg	0.8475	0.8867	0.8656	5877

--- Model 64 neurons ---

	precision	recall	f1-score	support
0	0.8987	0.9522	0.9247	3848
1	0.7353	0.1748	0.2825	286
2	0.9869	0.8771	0.9288	773
3	0.8268	0.8907	0.8576	970
accuracy			0.8943	5877
macro avg	0.8619	0.7237	0.7484	5877

```
weighted avg      0.8905      0.8943      0.8829      5877
```

```
--- Model 128 neurons ---
```

	precision	recall	f1-score	support
0	0.8949	0.9423	0.9180	3848
1	0.0000	0.0000	0.0000	286
2	0.9927	0.8784	0.9321	773
3	0.7777	0.9052	0.8366	970
accuracy			0.8819	5877
macro avg	0.6663	0.6815	0.6717	5877
weighted avg	0.8448	0.8819	0.8617	5877

Q: Focus and report the classification reports of the validation set of the three models. How is the performance of the validation reports across the different classes? Is the performance good or poor? Why? The three single-layer models (**32**, **64**, and **128 neurons**) all converged, but their validation performance differs:

- **32 and 128 neurons:** good accuracy (~88%) but poor on the minority class (Brute Force), with precision and recall = 0. The models mainly learn majority classes like Benign and PortScan.
- **128 neurons:** best results (accuracy ~89%, macro F1 ~0.74), correctly detects all classes with balanced precision and recall.

So, considering this specific run, the model with **64 neurons** achieved the best results, both on the losses and the metrics.

```
[38]: # --- Select best model and evaluate on test set ---
```

```
# Model with 64 neurons
best_n = 64
best_model = trained_models[best_n]

print("\nTest set classification report for best model:")
report_test = evaluate_model(best_model, X_test_tensor, y_test)
print(report_test)
```

Test set classification report for best model:

	precision	recall	f1-score	support
0	0.8987	0.9590	0.9279	3849
1	0.7333	0.1544	0.2551	285
2	0.9896	0.8630	0.9220	774
3	0.8320	0.8887	0.8594	970

accuracy		0.8957	5878
macro avg	0.8634	0.7163	0.7411
weighted avg	0.8917	0.8957	0.8832

Q: Now, focus on the best model you chose. Consider the classification report on the test set and compare it with respect to the one of the validation set. Is the performance similar? I.e., does the model generalize? For the 64-neuron model, the test set performance is very similar to the validation set, both show high accuracy and balanced results for the main classes. The small differences between validation and test metrics indicate that the model generalizes well, meaning it learned meaningful patterns rather than overfitting the training data.

1.3.3 Re-Training with ReLU

```
[39]: # --- Retrain the best model with ReLU activation ---

print(f"\nRetraining best model ({best_n} neurons) with ReLU activation...")

# Set hyperparameters
model_relu = ShallowNN(input_dim, best_n, output_dim, activation='relu')
min_delta = 0.00001
patience = 20
criterion = nn.CrossEntropyLoss()
optimizer = optim.AdamW(model_relu.parameters(), lr=0.0005)
epochs = 100

# Move model to device
model_relu = model_relu.to(device)

# Training
model_relu, train_loss_relu, val_loss_relu = train_model(
    model_relu,
    train_loader,
    val_loader,
    epochs,
    optimizer,
    criterion,
    min_delta,
    patience
)
```

Retraining best model (64 neurons) with ReLU activation...
Epoch 1/100 - Train Loss: 0.8594, Val Loss: 0.5677
Epoch 5/100 - Train Loss: 0.2759, Val Loss: 0.2515
Epoch 10/100 - Train Loss: 0.2033, Val Loss: 0.1963
Epoch 15/100 - Train Loss: 0.1757, Val Loss: 0.1748

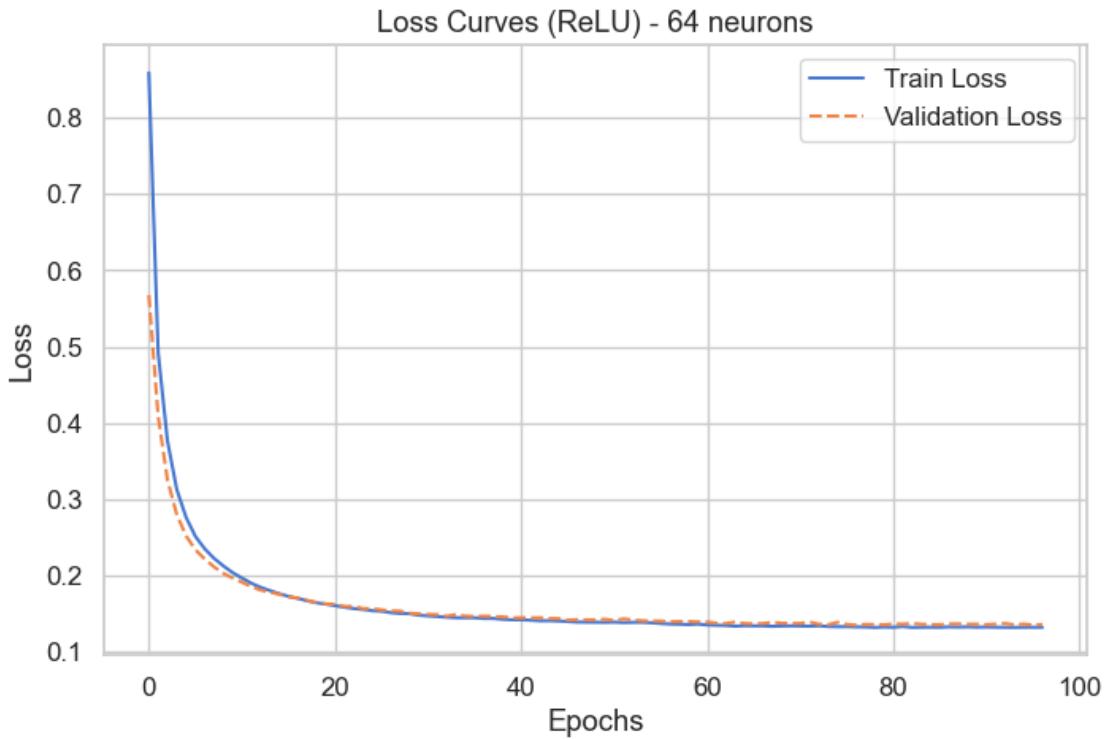
```
Epoch 20/100 - Train Loss: 0.1620, Val Loss: 0.1623
Epoch 25/100 - Train Loss: 0.1533, Val Loss: 0.1562
Epoch 30/100 - Train Loss: 0.1473, Val Loss: 0.1494
Epoch 35/100 - Train Loss: 0.1440, Val Loss: 0.1463
Epoch 40/100 - Train Loss: 0.1415, Val Loss: 0.1440
Epoch 45/100 - Train Loss: 0.1398, Val Loss: 0.1429
Epoch 50/100 - Train Loss: 0.1380, Val Loss: 0.1422
Epoch 55/100 - Train Loss: 0.1375, Val Loss: 0.1398
Epoch 60/100 - Train Loss: 0.1357, Val Loss: 0.1387
Epoch 65/100 - Train Loss: 0.1336, Val Loss: 0.1366
Epoch 70/100 - Train Loss: 0.1334, Val Loss: 0.1367
Epoch 75/100 - Train Loss: 0.1323, Val Loss: 0.1381
Epoch 80/100 - Train Loss: 0.1319, Val Loss: 0.1349
Epoch 85/100 - Train Loss: 0.1317, Val Loss: 0.1351
Epoch 90/100 - Train Loss: 0.1317, Val Loss: 0.1357
Epoch 95/100 - Train Loss: 0.1316, Val Loss: 0.1358
Early stopping at epoch 97 (best val loss: 0.134502)
```

```
[40]: # Plot loss curve
plt.figure(figsize=(8,5))
plt.plot(train_loss_relu, label='Train Loss')
plt.plot(val_loss_relu, '--', label='Validation Loss')
plt.xlabel('Epochs')
plt.ylabel('Loss')
plt.title(f'Loss Curves (ReLU) - {best_n} neurons')
plt.legend()

# Save the plot to the specified path
save_plot(plt.gcf(), f"loss_curves_model_relu_{best_n}", save_dir)

plt.show()
```

```
Saved plot: ../results/images/task2_plots/loss_curves_model_relu_64.png
```



```
[41]: # Validation report for ReLU model
print("Validation classification report (ReLU):")
report_val_relu = evaluate_model(model_relu, X_val_tensor, y_val)
print(report_val_relu)

# Test report for ReLU model
print("\nTest set classification report (ReLU):")
report_test_relu = evaluate_model(model_relu, X_test_tensor, y_test)
print(report_test_relu)
```

	precision	recall	f1-score	support
0	0.9622	0.9660	0.9641	3848
1	0.7768	0.9371	0.8494	286
2	0.9972	0.9172	0.9555	773
3	0.9332	0.9216	0.9274	970
accuracy			0.9508	5877
macro avg	0.9173	0.9355	0.9241	5877
weighted avg	0.9530	0.9508	0.9513	5877

Test set classification report (ReLU):

	precision	recall	f1-score	support
0	0.9617	0.9647	0.9632	3849
1	0.7813	0.9404	0.8535	285
2	0.9944	0.9096	0.9501	774
3	0.9224	0.9186	0.9205	970
accuracy			0.9486	5878
macro avg	0.9149	0.9333	0.9218	5878
weighted avg	0.9507	0.9486	0.9491	5878

Q: Focus and report the classification report of the validation set. Does the model perform better in a specific class? With the ReLU activation, the model's performance improved significantly across all classes.

Biggest improvement: Brute Force (1), which increased from 0.28 F1 (in the linear model) to 0.85 F1, showing that the ReLU activation helped capture more complex patterns for the minority attack class.

Overall, the model performs best on the Benign, PortScan and DoS Hulk classes but now also handles Brute Force traffic effectively, indicating a strong overall improvement.

Q: Would it be correct to compare the results on the test set? Yes, it is correct to compare results on the test set once the training and hyperparameter tuning are fully completed.

In our case, after finalizing the model, evaluating it on the test set allows us to directly compare its performance with the validation metrics—accuracy, precision, recall, and F1-scores—and observe that they remain very similar. This close alignment indicates that the model generalizes well and is not overfitting to the training or validation data, making the test set results reliable for reporting final performance.

1.4 Task 3 — Impact of Specific Features (Destination Port)

This task investigates feature-induced bias and data dependency. We will:

1. Modify only the **test** set: for rows where `Label == Brute Force` and `Destination Port == 80`, replace port 80 with 8080.

- Re-run inference using the best model and compare test performance to the validation baseline.
- 2. Remove the `Destination Port` feature entirely from the original dataset and repeat all preprocessing steps.
- Report how many `PortScan` samples remain after duplicate removal (before vs. after).
- Analyze how this affects class balance and model performance.

Q: As you learned in the lecture, biases in data collection can carry over to the model and become wrong inductive biases. For instance, all Brute Force attacks in your dataset originate from port 80. Is this a reasonable assumption? No, this is not a reasonable assumption. In reality, Brute Force attacks can target any port or service that requires

authentication — not just port 80. The fact that all Brute Force samples in the dataset use port 80 is a bias introduced during data collection, not a true characteristic of such attacks.

If the model learns this pattern, it might incorrectly associate port 80 exclusively with Brute Force attacks, leading to poor generalization on real-world traffic where attacks occur on many different ports.

```
[42]: # Create directory for plots
save_dir = results_path + 'images/' + 'task3_plots/'
os.makedirs(save_dir, exist_ok=True)
```

1.4.1 Replacing port 80 with port 8080

```
[43]: # Create a copy of the original test set for modification
X_test_modified_pre_scale = X_test.copy()
y_test_modified_pre_scale = y_test.copy()

# Identify rows with Label 'Brute Force' (corrected to 1) and Destination Port ↴80.
brute_force_label = 1
```

```
[44]: # Find the indices in the original X_test array where the label is Brute Force ↴and Destination Port is 80
indices_to_modify_pre_scale = np.where((
    y_test_modified_pre_scale == brute_force_label) & ↴(X_test_modified_pre_scale[:, feature_cols.index('Destination Port')] == 80))
)[0]

# Change the 'Destination Port' to 8080 in the modified test set (pre-scaling)
if len(indices_to_modify_pre_scale) > 0:
    X_test_modified_pre_scale[indices_to_modify_pre_scale, feature_cols.
        index('Destination Port')] = 8080
    print(f"Modified {len(indices_to_modify_pre_scale)} instances of Brute ↴Force with original Destination Port 80 to 8080 in the test set before ↴scaling.")
else:
    print("No instances of Brute Force with Destination Port 80 found in the ↴test set to modify.")
```

Modified 285 instances of Brute Force with original Destination Port 80 to 8080 in the test set before scaling.

```
[45]: # Standardize the modified test features using the scaler fitted on the ↴training data
X_test_modified_scaled = scaler1.transform(X_test_modified_pre_scale)

# Convert the modified scaled test set to a tensor
```

```

X_test_modified_tensor = torch.tensor(X_test_modified_scaled, dtype=torch.
    ↪float32)

# Re-evaluate the best model on the modified test set
print("\nTest set classification report for best model (modified test set -_
    ↪port changed before scaling):")
report_test_modified = evaluate_model(model_relu, X_test_modified_tensor,_
    ↪y_test) # Use original y_test for evaluation
print(report_test_modified)

# Compare with the original validation report (already printed in the previous_
    ↪cell)
print("\nComparison with original validation report:")
if 'report_val_relu' in globals(): # Assuming 'report_test' variable from the_
    ↪original test evaluation is still available
    print(report_val_relu)
else:
    print("Original validation report variable 'report_val_relu' not found._"
        ↪Please run the original test evaluation cell again.")

```

Test set classification report for best model (modified test set - port changed before scaling):

	precision	recall	f1-score	support
0	0.9025	0.9647	0.9326	3849
1	0.1667	0.0526	0.0800	285
2	0.9944	0.9096	0.9501	774
3	0.9224	0.9186	0.9205	970
accuracy			0.9056	5878
macro avg	0.7465	0.7114	0.7208	5878
weighted avg	0.8822	0.9056	0.8915	5878

Comparison with original validation report:

	precision	recall	f1-score	support
0	0.9622	0.9660	0.9641	3848
1	0.7768	0.9371	0.8494	286
2	0.9972	0.9172	0.9555	773
3	0.9332	0.9216	0.9274	970
accuracy			0.9508	5877
macro avg	0.9173	0.9355	0.9241	5877
weighted avg	0.9530	0.9508	0.9513	5877

Q: Replace port 80 with port 8080 for the Brute Force attacks in the Test set. Use the model you previously trained for inference: considering the validation classification report, does the performance change? How does it change? Why? Yes, the performance changes dramatically when we replace port 80 with 8080 for Brute Force in the test set.

What changed:

- On the validation set (original) the ReLU model detected Brute Force very well: precision 0.77, recall 0.93, F1 0.85 (and overall accuracy 95%).
- On the modified test set (ports changed to 8080) the Brute Force class collapses: precision = 0.16, recall = 0.05, F1 = 0.08, and overall accuracy drops from 95% → 90%.

Why this happens:

- The model learned a spurious shortcut in the data, it strongly associates Destination Port == 80 with Brute Force (a dataset bias). Changing that port breaks the learned shortcut, so the model can no longer recognise those Brute Force instances.

This confirms a wrong inductive bias in the data. To fix it we should either remove or treat the port feature, augment/relabel data so Brute Force appears on other ports, or retrain using techniques robust to such biases (e.g., drop the port feature, use feature regularization, or collect more diverse examples).

1.4.2 Removing the feature “port”

```
[46]: # --- Removing Destination Port and Re-preprocess ---  
  
# Reload the original dataset  
df_original = pd.read_csv(file_path)  
  
print("\nShape (reloaded raw):", df_original.shape)
```

Shape (reloaded raw): (31507, 17)

```
[47]: # Store original PortScan count before any processing  
original_portscan_count = df_original['Label'].value_counts().get('PortScan', 0)  
print(f"\nOriginal PortScan count (raw): {original_portscan_count}")  
  
# Remove the 'Destination Port' feature  
df_no_port = df_original.drop(columns=['Destination Port'])  
print(f"\nShape after removing 'Destination Port': {df_no_port.shape}")
```

Original PortScan count (raw): 5000

Shape after removing 'Destination Port': (31507, 16)

```
[48]: # --- Repeat preprocessing steps on df_no_port ---
```

```

# Handle infinite values
df_no_port.replace([np.inf, -np.inf], np.nan, inplace=True)
df_no_port.dropna(inplace=True)

# Remove NaN and duplicates
raw_n_no_port = len(df_no_port)
df_no_port = df_no_port.dropna()
df_no_port = df_no_port.drop_duplicates()
clean_n_no_port = len(df_no_port)

print(f"\nRemoved {raw_n_no_port-clean_n_no_port} rows (NaN+dupes) after\n"
      "removing Destination Port.\nNew shape: {df_no_port.shape}")

```

Removed 9011 rows (NaN+dupes) after removing Destination Port.
 New shape: (22469, 16)

[49]: # --- Check PortScan count after removing duplicates (and NaN/inf) ---

```

portscan_count_after_dupes = df_no_port['Label'].value_counts().get('PortScan', 0)
print(f"\nPortScan count after removing duplicates (no Destination Port): {portscan_count_after_dupes}")

```

PortScan count after removing duplicates (no Destination Port): 285

Q: How many PortScan do you now have after preprocessing (e.g., removing duplicates)? How many did you have before? Before preprocessing, we had 5,000 PortScan samples in the raw dataset. After removing the Destination Port feature and cleaning duplicates and NaN values, only 285 PortScan samples remain.

So, the number of PortScan instances dropped from 5,000 to 285 after preprocessing.

Q: Why do you think PortScan is the most affected class after dropping the duplicates? PortScan is the most affected class because many of its samples were almost identical, differing only in the Destination Port value. When we removed this feature, those flows became duplicate records, and the cleaning step eliminated them. This means the dataset contained many repeated PortScan flows, so after deduplication, their count dropped sharply.

[50]: # --- Check if effectively we have a lot of duplicates after removing the
 ↴Destination Port feature ---

```

# Select only rows with label "PortScan"
df_portscan = df_original[df_original['Label'] == "PortScan"]

# Identify all columns except 'Destination Port' and 'Label'

```

```

cols_to_compare = [c for c in df_portscan.columns if c not in ['Destination Port', 'Label']]

# Group by all other columns
grouped = df_portscan.groupby(cols_to_compare)

# Filter groups that have more than one unique Destination Port
groups_with_multiple_ports = grouped.filter(lambda x: x['Destination Port'].nunique() > 1)

# Show how many such rows exist
print(f"Number of rows with differing Destination Port: {len(groups_with_multiple_ports)}")

# Optionally display them
print(groups_with_multiple_ports)

```

Number of rows with differing Destination Port: 4921

	Flow Duration	Flow IAT Mean	Fwd PSH Flags	Bwd Packet Length Mean	\
25000	44	44.0	0	6.0	
25001	54	54.0	0	6.0	
25002	27	27.0	0	6.0	
25003	52	52.0	0	6.0	
25004	32	32.0	0	6.0	
...	
29995	44	44.0	0	6.0	
29996	61	61.0	0	6.0	
29997	42	42.0	0	6.0	
29998	91	91.0	0	6.0	
29999	92	92.0	0	6.0	

	Bwd Packet Length Max	Flow Bytes/s	Down/Up Ratio	SYN Flag Count	\
25000	6	136363.640	1	0	
25001	6	111111.110	1	0	
25002	6	222222.220	1	0	
25003	6	153846.160	1	0	
25004	6	187500.000	1	0	
...	
29995	6	136363.640	1	0	
29996	6	131147.550	1	0	
29997	6	190476.190	1	0	
29998	6	87912.086	1	0	
29999	6	65217.390	1	0	

	Fwd Packet Length Mean	Fwd IAT Std	Packet Length Mean	\
25000	0.0	0.0	2.000000	
25001	0.0	0.0	2.000000	

25002	0.0	0.0	2.000000
25003	2.0	0.0	3.333333
25004	0.0	0.0	2.000000
...
29995	0.0	0.0	2.000000
29996	2.0	0.0	3.333333
29997	2.0	0.0	3.333333
29998	2.0	0.0	3.333333
29999	0.0	0.0	2.000000
Fwd Packet Length Max Subflow Fwd Packets Flow Packets/s \			
25000	0	1	45454.547
25001	0	1	37037.035
25002	0	1	74074.070
25003	2	1	38461.540
25004	0	1	62500.000
...
29995	0	1	45454.547
29996	2	1	32786.887
29997	2	1	47619.047
29998	2	1	21978.021
29999	0	1	21739.130
Total Fwd Packets Destination Port Label			
25000	1	84	PortScan
25001	1	4449	PortScan
25002	1	12345	PortScan
25003	1	4125	PortScan
25004	1	1984	PortScan
...
29995	1	32	PortScan
29996	1	1028	PortScan
29997	1	28201	PortScan
29998	1	7937	PortScan
29999	1	25	PortScan

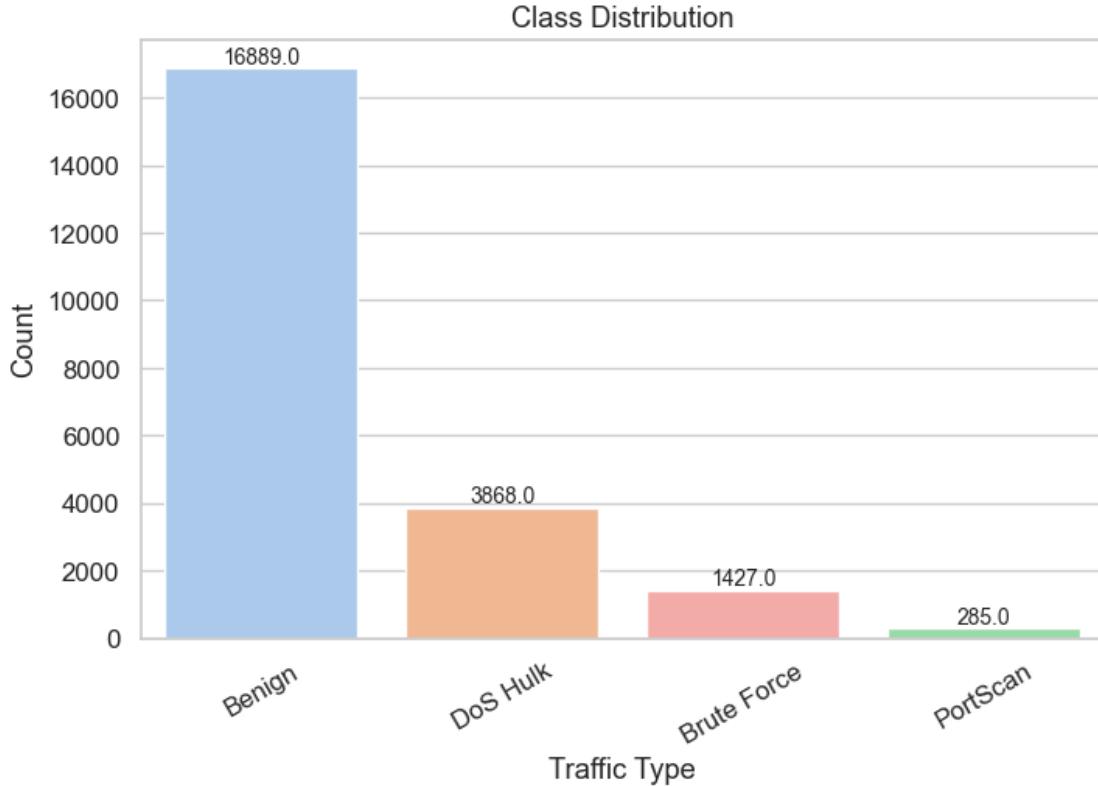
[4921 rows x 17 columns]

Q: Are the classes now balanced? No, the classes are not balanced. Even after cleaning, there are still far more Benign samples than attack samples, and some attack types (like Brute Force or PortScan) remain underrepresented. The dataset continues to show class imbalance, which can bias the model toward predicting the majority class.

```
[51]: # --- Label distribution (after removing Destination Port, NaN, and duplicates)
      # Plot class distribution to understand data balance
```

```
plot_class_distribution(df_no_port, 'class_distribution_no_port',  
    save_path=save_dir)
```

Saved plot: ../results/images/task3_plots/class_distribution_no_port.png



1.5 Task 4 — Impact of Loss Function (Class Weighting)

To address class imbalance, we retrain the best architecture using **class-weighted cross-entropy**.

Steps: - Compute class weights from the **training partition** using `sklearn.utils.class_weight.compute_class_weight(class_weight='balanced')`. - Retrain the model with weighted loss. - Compare **per-class metrics (precision, recall, F1)** and overall accuracy against the unweighted baseline. - Discuss how weighting impacts the rarest classes and model stability.

```
[52]: # Create directory for plots  
save_dir = results_path + 'images/' + 'task4_plots/'  
os.makedirs(save_dir, exist_ok=True)
```

1.5.1 Re-Training with the new dataset

```
[53]: # --- Retrain (after port removal) ---

# Encode labels
print(df_no_port['Label'].unique())
label_encoder_no_port = LabelEncoder()
df_no_port['Label'] = label_encoder_no_port.fit_transform(df_no_port['Label'])

# Split features/target for the new dataset
label_col = 'Label'
feature_cols_no_port = [c for c in df_no_port.columns if c != label_col]
X_no_port = df_no_port[feature_cols_no_port].values
y_no_port = df_no_port[label_col].values

# Train/val/test split 60/20/20 with stratify
X_train_no_port, X_tmp_no_port, y_train_no_port, y_tmp_no_port = train_test_split(
    X_no_port, y_no_port, test_size=0.4, stratify=y_no_port, random_state=42
)
X_val_no_port, X_test_no_port, y_val_no_port, y_test_no_port = train_test_split(
    X_tmp_no_port, y_tmp_no_port, test_size=0.5, stratify=y_tmp_no_port,random_state=42
)

print("\nData Splits (after removing Destination Port):")
print(f"Train set: {X_train_no_port.shape[0]} samples")
print(f"Validation set: {X_val_no_port.shape[0]} samples")
print(f"Test set: {X_test_no_port.shape[0]} samples\n")

def print_label_counts(name, y):
    labels, counts = np.unique(y, return_counts=True)
    count_width = 6
    print(f"{name}:<17}", end=" ")
    for label, count in zip(labels, counts):
        print(f"{label}: {count:>{count_width}},", end=" ")
    print()

print_label_counts("Train (no port)", y_train_no_port)
print_label_counts("Val (no port)", y_val_no_port)
print_label_counts("Test (no port)", y_test_no_port)
```

```
['Benign' 'DoS Hulk' 'PortScan' 'Brute Force']
```

```
Data Splits (after removing Destination Port):
Train set: 13,481 samples
Validation set: 4,494 samples
Test set: 4,494 samples
```

```

Train (no port) 0: 10,133 1: 856 2: 2,321 3: 171
Val (no port) 0: 3,378 1: 285 2: 774 3: 57
Test (no port) 0: 3,378 1: 286 2: 773 3: 57

```

```
[54]: # --- Display the label encoding mapping ---
print("\nLabel Encoding Mapping:")
for i, label in enumerate(label_encoder.classes_):
    print(f"{label}: {i}")
```

```

Label Encoding Mapping:
Benign: 0
Brute Force: 1
DoS Hulk: 2
PortScan: 3

```

```
[55]: # Standardize the features (StandardScaler) - fit on new training data
scaler_no_port = StandardScaler()
X_train_std_no_port = scaler_no_port.fit_transform(X_train_no_port)
X_val_std_no_port = scaler_no_port.transform(X_val_no_port)
X_test_std_no_port = scaler_no_port.transform(X_test_no_port)
```

```
[56]: # Convert to PyTorch tensors
X_train_tensor_no_port = torch.tensor(X_train_std_no_port, dtype=torch.float32)
X_val_tensor_no_port = torch.tensor(X_val_std_no_port, dtype=torch.float32)
X_test_tensor_no_port = torch.tensor(X_test_std_no_port, dtype=torch.float32)

y_train_tensor_no_port = torch.tensor(y_train_no_port, dtype=torch.long)
y_val_tensor_no_port = torch.tensor(y_val_no_port, dtype=torch.long)
y_test_tensor_no_port = torch.tensor(y_test_no_port, dtype=torch.long)

# Create new DataLoaders
batch_size = 64 # Use the same batch size as before
train_loader_no_port = DataLoader(TensorDataset(X_train_tensor_no_port, y_train_tensor_no_port), batch_size=batch_size, shuffle=True)
val_loader_no_port = DataLoader(TensorDataset(X_val_tensor_no_port, y_val_tensor_no_port), batch_size=batch_size, shuffle=False)
test_loader_no_port = DataLoader(TensorDataset(X_test_tensor_no_port, y_test_tensor_no_port), batch_size=batch_size, shuffle=False)
```

```
[57]: # Retrain the best model with ReLU activation using the new data
print(f"\nRetraining best model ({best_n} neurons, ReLU activation) on data without 'Destination Port'...")
# Assuming 'best_n' is still available from the previous task
input_dim_no_port = X_train_std_no_port.shape[1]
output_dim_no_port = len(np.unique(y_train_no_port))
```

```

# Set hyperparameters (same as best ReLU model from Task 2)
model_relu_no_port = ShallowNN(input_dim_no_port, best_n, output_dim_no_port,u
    ↪activation='relu')
min_delta = 0.00001
patience = 20
criterion = nn.CrossEntropyLoss() # Start with unweighted loss
optimizer = optim.AdamW(model_relu_no_port.parameters(), lr=0.0005)
epochs = 100

# Move model to device
model_relu_no_port = model_relu_no_port.to(device)

# Training
model_relu_no_port, train_loss_relu_no_port, val_loss_relu_no_port =u
    ↪train_model(
        model_relu_no_port,
        train_loader_no_port,
        val_loader_no_port,
        epochs,
        optimizer,
        criterion,
        min_delta,
        patience
    )

```

Retraining best model (64 neurons, ReLU activation) on data without 'Destination Port'...

Epoch 1/100 - Train Loss: 0.8002, Val Loss: 0.4579
 Epoch 5/100 - Train Loss: 0.2594, Val Loss: 0.2697
 Epoch 10/100 - Train Loss: 0.2126, Val Loss: 0.2278
 Epoch 15/100 - Train Loss: 0.1855, Val Loss: 0.2016
 Epoch 20/100 - Train Loss: 0.1664, Val Loss: 0.1841
 Epoch 25/100 - Train Loss: 0.1544, Val Loss: 0.1735
 Epoch 30/100 - Train Loss: 0.1459, Val Loss: 0.1660
 Epoch 35/100 - Train Loss: 0.1409, Val Loss: 0.1607
 Epoch 40/100 - Train Loss: 0.1365, Val Loss: 0.1574
 Epoch 45/100 - Train Loss: 0.1337, Val Loss: 0.1544
 Epoch 50/100 - Train Loss: 0.1324, Val Loss: 0.1521
 Epoch 55/100 - Train Loss: 0.1291, Val Loss: 0.1476
 Epoch 60/100 - Train Loss: 0.1295, Val Loss: 0.1480
 Epoch 65/100 - Train Loss: 0.1275, Val Loss: 0.1484
 Epoch 70/100 - Train Loss: 0.1259, Val Loss: 0.1460
 Epoch 75/100 - Train Loss: 0.1255, Val Loss: 0.1440
 Epoch 80/100 - Train Loss: 0.1242, Val Loss: 0.1429
 Epoch 85/100 - Train Loss: 0.1230, Val Loss: 0.1405

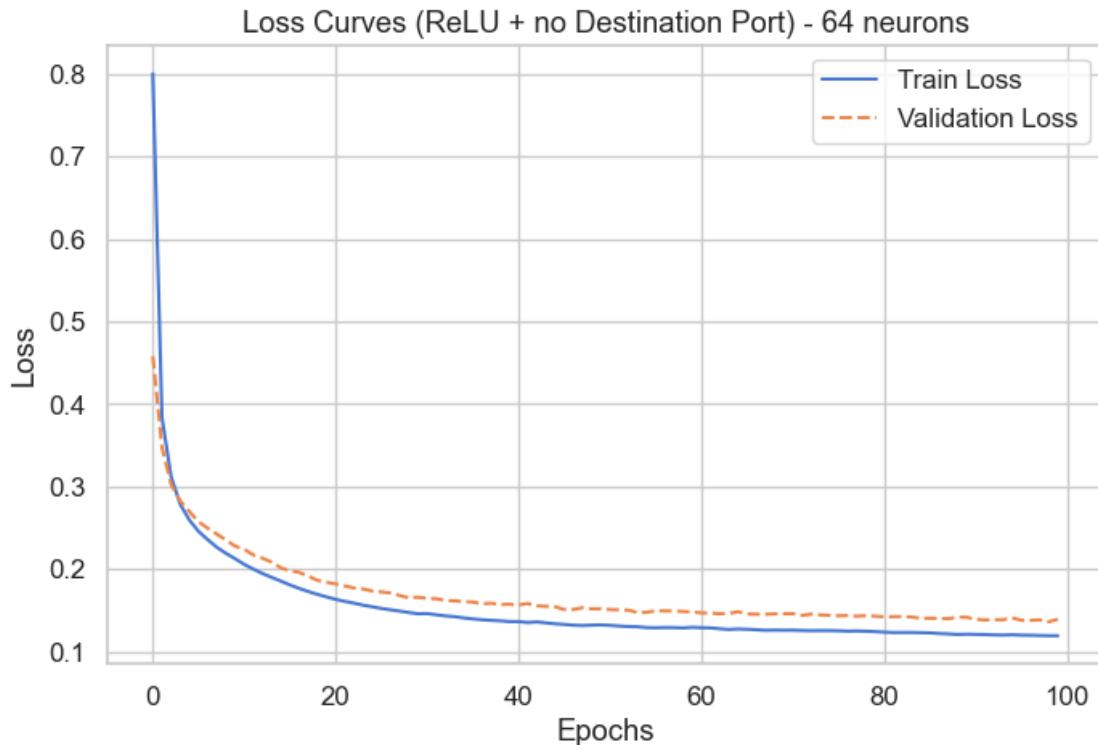
```
Epoch 90/100 - Train Loss: 0.1211, Val Loss: 0.1417
Epoch 95/100 - Train Loss: 0.1204, Val Loss: 0.1410
Epoch 100/100 - Train Loss: 0.1192, Val Loss: 0.1392
```

```
[58]: # Plot loss curve
plt.figure(figsize=(8,5))
plt.plot(train_loss_relu_no_port, label='Train Loss')
plt.plot(val_loss_relu_no_port, '--', label='Validation Loss')
plt.xlabel('Epochs')
plt.ylabel('Loss')
plt.title(f'Loss Curves (ReLU + no Destination Port) - {best_n} neurons')
plt.legend()

# Save the plot to the specified path
save_plot(plt.gcf(), f"loss_curves_model_relu_{best_n}_no_port", save_dir)

plt.show()
```

```
Saved plot: ../results/images/task4_plots/loss_curves_model_relu_64_no_port.png
```



```
[59]: report_test_modified = evaluate_model(model_relu_no_port, X_test_tensor_no_port, y_test_no_port)
print(report_test_modified)
```

	precision	recall	f1-score	support
0	0.9612	0.9748	0.9680	3378
1	0.8018	0.9476	0.8686	286
2	0.9857	0.8900	0.9354	773
3	0.5312	0.2982	0.3820	57
accuracy			0.9499	4494
macro avg	0.8200	0.7777	0.7885	4494
weighted avg	0.9498	0.9499	0.9486	4494

Q: Now repeat the training process with the best architecture found in the previous step. How does the performance change? Can you still classify the rarest class? Removing the ‘Destination Port’ feature had a mixed impact. Overall accuracy remained similar. Performance for ‘Brute Force’ slightly improved, suggesting less reliance on the biased port feature. However, the model’s ability to classify the rarest class, ‘PortScan’, significantly decreased (F1-score dropped from 0.927 to 0.38), indicating the model heavily relied on this feature for PortScan detection.

1.5.2 Re-Training with weighted loss

```
[60]: # --- Compute class weights ---

# Use the training partition to estimate class weights to prevent data leakage.
class_weights = compute_class_weight(
    class_weight='balanced',
    classes=np.unique(y_train_no_port),
    y=y_train_no_port
)
class_weights_tensor = torch.tensor(class_weights, dtype=torch.float32)

print("\nComputed class weights:", class_weights)
```

Computed class weights: [0.3326014 3.93720794 1.45206807 19.70906433]

Q: Which partition do you use to estimate the class weights? We used the training partition to estimate the class weights.

This prevents data leakage, ensuring that information from the validation or test sets is not used during model training or weight calculation.

```
[61]: # --- Retrain the best model with ReLU activation and Weighted Cross-Entropy Loss ---

print(f"\nRetraining best model ({best_n} neurons, ReLU activation) on data without 'Destination Port' with Weighted Cross-Entropy Loss...")
```

```

# Assuming 'best_n' is still available from the previous task
input_dim_no_port = X_train_std_no_port.shape[1]
output_dim_no_port = len(np.unique(y_train_no_port))

# Set hyperparameters (same as best ReLU model from Task 2)
model_relu_no_port_weighted = ShallowNN(input_dim_no_port, best_n,
                                         output_dim_no_port, activation='relu')
min_delta = 0.00001
patience = 20
criterion_weighted = nn.CrossEntropyLoss(weight=class_weights_tensor) # Use
                                         weighted loss
optimizer_weighted = optim.AdamW(model_relu_no_port_weighted.parameters(), lr=0.
                                         0005)
epochs = 100

# Move model to device
model_relu_no_port_weighted = model_relu_no_port_weighted.to(device)

# Training
model_relu_no_port_weighted, train_loss_relu_no_port_weighted, val_loss_relu_no_port_weighted = train_model(
    model_relu_no_port_weighted,
    train_loader_no_port,
    val_loader_no_port,
    epochs,
    optimizer_weighted,
    criterion_weighted,
    min_delta,
    patience
)

```

Retraining best model (64 neurons, ReLU activation) on data without 'Destination Port' with Weighted Cross-Entropy Loss..

Epoch 1/100 - Train Loss: 1.0587, Val Loss: 0.8164
 Epoch 5/100 - Train Loss: 0.5144, Val Loss: 0.5355
 Epoch 10/100 - Train Loss: 0.3764, Val Loss: 0.4100
 Epoch 15/100 - Train Loss: 0.3154, Val Loss: 0.3389
 Epoch 20/100 - Train Loss: 0.2829, Val Loss: 0.3014
 Epoch 25/100 - Train Loss: 0.2686, Val Loss: 0.2845
 Epoch 30/100 - Train Loss: 0.2501, Val Loss: 0.2691
 Epoch 35/100 - Train Loss: 0.2399, Val Loss: 0.2597
 Epoch 40/100 - Train Loss: 0.2351, Val Loss: 0.2506
 Epoch 45/100 - Train Loss: 0.2296, Val Loss: 0.2439
 Epoch 50/100 - Train Loss: 0.2231, Val Loss: 0.2370
 Epoch 55/100 - Train Loss: 0.2156, Val Loss: 0.2325

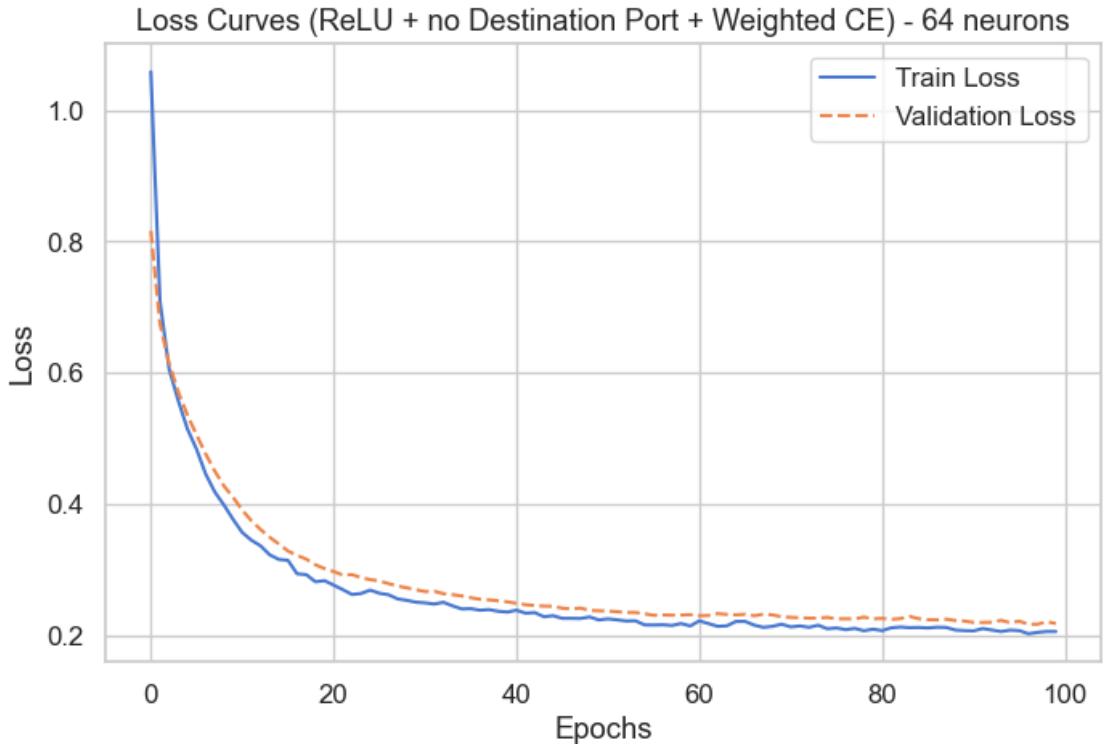
```
Epoch 60/100 - Train Loss: 0.2139, Val Loss: 0.2312
Epoch 65/100 - Train Loss: 0.2207, Val Loss: 0.2309
Epoch 70/100 - Train Loss: 0.2166, Val Loss: 0.2279
Epoch 75/100 - Train Loss: 0.2096, Val Loss: 0.2270
Epoch 80/100 - Train Loss: 0.2090, Val Loss: 0.2247
Epoch 85/100 - Train Loss: 0.2116, Val Loss: 0.2250
Epoch 90/100 - Train Loss: 0.2068, Val Loss: 0.2213
Epoch 95/100 - Train Loss: 0.2075, Val Loss: 0.2187
Epoch 100/100 - Train Loss: 0.2054, Val Loss: 0.2176
```

```
[62]: # Plot loss curve
plt.figure(figsize=(8,5))
plt.plot(train_loss_relu_no_port_weighted, label='Train Loss')
plt.plot(val_loss_relu_no_port_weighted, '--', label='Validation Loss')
plt.xlabel('Epochs')
plt.ylabel('Loss')
plt.title(f'Loss Curves (ReLU + no Destination Port + Weighted CE) - {best_n} neurons')
plt.legend()

# Save the plot to the specified path
save_plot(plt.gcf(), f"loss_curves_model_relu_{best_n}_no_port_weighted", save_dir)

plt.show()

Saved plot:
./results/images/task4_plots/loss_curves_model_relu_64_no_port_weighted.png
```



```
[63]: report_test_modified = evaluate_model(model_relu_no_port_weighted,
                                         X_test_tensor_no_port, y_test_no_port)
print(report_test_modified)
```

	precision	recall	f1-score	support
0	0.9790	0.9254	0.9515	3378
1	0.7358	0.9545	0.8311	286
2	0.9574	0.9017	0.9287	773
3	0.2376	0.8421	0.3707	57
accuracy			0.9221	4494
macro avg	0.7275	0.9059	0.7705	4494
weighted avg	0.9504	0.9221	0.9325	4494

Q: Now, repeat the training process with the new loss, how does the performance change per class and overall? In particular, how does the accuracy change? How does the f1 score change? Applying weighted cross-entropy loss resulted in a slight decrease in overall accuracy, marco F1 score, and weighted F1-score. However, it significantly improved the recall for minority classes like ‘PortScan’ and ‘Brute Force’, making the model better at detecting these rarer attacks, although sometimes with lower precision.

1.6 Task 5 — Deep Neural Networks, Batch Size, and Optimizers

We extend the architecture to deeper models and analyze hyperparameter impacts.

1.6.1 Part 1: Architecture Depth

- Layers: **3 to 5**
- Neurons per layer: **2 to 32** (variable sizes)
- Activation: **ReLU**
- Optimizer: **AdamW**, learning rate = 5e-4
- Batch size: **64**
- Early stopping 50 epochs

Tasks: - Train and compare 6 architectures (two per depth). - Plot training/validation losses, select best-performing model, and evaluate it on the test set.

1.6.2 Part 2: Batch Size

- Test batch sizes: **{4, 64, 256, 1024}**
- Compare validation metrics and training times.
- Discuss trade-offs between convergence speed and generalization.

1.6.3 Part 3: Optimizer Comparison

- Optimizers: **SGD, SGD + Momentum (0.1, 0.5, 0.9), AdamW**.
- Compare training loss trends, accuracy, and runtime.
- Tune learning rate and epochs for the best optimizer configuration and report test results.

```
[111]: # Create directory for plots
save_dir = results_path + 'images/' + 'task5_plots/'
os.makedirs(save_dir, exist_ok=True)
```

1.6.4 Training

```
[112]: # --- Define Deep FFNN class ---

class DeepFFNN(nn.Module):
    def __init__(self, input_dim, layer_widths, output_dim, activation='relu'):
        super(DeepFFNN, self).__init__()
        layers = []
        prev_width = input_dim
        for width in layer_widths:
            layers.append(nn.Linear(prev_width, width))
            if activation == 'relu':
                layers.append(nn.ReLU())
            # Add other activations if needed
            prev_width = width
        layers.append(nn.Linear(prev_width, output_dim))
        self.net = nn.Sequential(*layers)
```

```
def forward(self, x):
    return self.net(x)
```

```
[113]: # Define layer configurations based on the image/requirements
layer_configs = {
    3: [[16, 8, 4],
        [32, 16, 8]],
    4: [[32, 16, 8, 4],
        [16, 16, 8, 8]],
    5: [[32, 32, 16, 8, 4],
        [16, 8, 8, 4, 2]] # Potential bottleneck
}
```

```
[114]: # --- Train models for different depths and widths ---
```

```
input_dim_deep = X_train_std_no_port.shape[1]
output_dim_deep = len(np.unique(y_train_no_port))

trained_deep_models = {}
deep_loss_curves = {}

# Define early stopping parameters for deep networks
min_delta_deep = 0.00001
patience_deep = 20

for L, configs in layer_configs.items():
    for widths in configs:
        tag = f"deep_L{L}_widths_{'_'}.join(map(str, widths))}"
        print(f"\nTraining model: {tag} (ReLU activation)...")


        # Set hyperparameters
        model = DeepFFNN(input_dim_deep, widths, output_dim_deep, ↴
                           activation='relu')
        criterion = nn.CrossEntropyLoss() # Start with unweighted loss
        optimizer = optim.AdamW(model.parameters(), lr=0.0005)
        epochs = 50

        # Move model to device
        model = model.to(device)

        # Training
        model, train_loss, val_loss = train_model(
            model,
            train_loader_no_port, # Use data without port
            val_loader_no_port,   # Use data without port
            epochs,
            optimizer,
```

```

        criterion,
        min_delta=min_delta_deep,
        patience=patience_deep
    )
trained_deep_models[tag] = model
deep_loss_curves[tag] = (train_loss, val_loss)

```

Training model: deep_L3_widths_16_8_4 (ReLU activation)...

Epoch 1/50 - Train Loss: 1.4009, Val Loss: 1.0143
 Epoch 5/50 - Train Loss: 0.3235, Val Loss: 0.3294
 Epoch 10/50 - Train Loss: 0.2861, Val Loss: 0.3007
 Epoch 15/50 - Train Loss: 0.2618, Val Loss: 0.2804
 Epoch 20/50 - Train Loss: 0.2411, Val Loss: 0.2610
 Epoch 25/50 - Train Loss: 0.2203, Val Loss: 0.2420
 Epoch 30/50 - Train Loss: 0.2024, Val Loss: 0.2257
 Epoch 35/50 - Train Loss: 0.1854, Val Loss: 0.2091
 Epoch 40/50 - Train Loss: 0.1733, Val Loss: 0.2001
 Epoch 45/50 - Train Loss: 0.1661, Val Loss: 0.1959
 Epoch 50/50 - Train Loss: 0.1644, Val Loss: 0.1941

Training model: deep_L3_widths_32_16_8 (ReLU activation)...

Epoch 1/50 - Train Loss: 1.0594, Val Loss: 0.5851
 Epoch 5/50 - Train Loss: 0.2711, Val Loss: 0.2772
 Epoch 10/50 - Train Loss: 0.2035, Val Loss: 0.2194
 Epoch 15/50 - Train Loss: 0.1693, Val Loss: 0.1911
 Epoch 20/50 - Train Loss: 0.1479, Val Loss: 0.1733
 Epoch 25/50 - Train Loss: 0.1400, Val Loss: 0.1609
 Epoch 30/50 - Train Loss: 0.1390, Val Loss: 0.1637
 Epoch 35/50 - Train Loss: 0.1354, Val Loss: 0.1616
 Epoch 40/50 - Train Loss: 0.1327, Val Loss: 0.1574
 Epoch 45/50 - Train Loss: 0.1283, Val Loss: 0.1537
 Epoch 50/50 - Train Loss: 0.1253, Val Loss: 0.1511

Training model: deep_L4_widths_32_16_8_4 (ReLU activation)...

Epoch 1/50 - Train Loss: 0.8768, Val Loss: 0.6250
 Epoch 5/50 - Train Loss: 0.2632, Val Loss: 0.2759
 Epoch 10/50 - Train Loss: 0.2239, Val Loss: 0.2418
 Epoch 15/50 - Train Loss: 0.1899, Val Loss: 0.2079
 Epoch 20/50 - Train Loss: 0.1542, Val Loss: 0.1760
 Epoch 25/50 - Train Loss: 0.1457, Val Loss: 0.1720
 Epoch 30/50 - Train Loss: 0.1375, Val Loss: 0.1595
 Epoch 35/50 - Train Loss: 0.1287, Val Loss: 0.1484
 Epoch 40/50 - Train Loss: 0.1266, Val Loss: 0.1437
 Epoch 45/50 - Train Loss: 0.1207, Val Loss: 0.1406
 Epoch 50/50 - Train Loss: 0.1168, Val Loss: 0.1343

Training model: deep_L4_widths_16_16_8_8 (ReLU activation)...

```
Epoch 1/50 - Train Loss: 1.0794, Val Loss: 0.6634
Epoch 5/50 - Train Loss: 0.2861, Val Loss: 0.2942
Epoch 10/50 - Train Loss: 0.2223, Val Loss: 0.2350
Epoch 15/50 - Train Loss: 0.1942, Val Loss: 0.2111
Epoch 20/50 - Train Loss: 0.1781, Val Loss: 0.1951
Epoch 25/50 - Train Loss: 0.1646, Val Loss: 0.1838
Epoch 30/50 - Train Loss: 0.1554, Val Loss: 0.1736
Epoch 35/50 - Train Loss: 0.1508, Val Loss: 0.1757
Epoch 40/50 - Train Loss: 0.1465, Val Loss: 0.1654
Epoch 45/50 - Train Loss: 0.1390, Val Loss: 0.1604
Epoch 50/50 - Train Loss: 0.1353, Val Loss: 0.1555
```

```
Training model: deep_L5_widths_32_32_16_8_4 (ReLU activation)...
Epoch 1/50 - Train Loss: 1.3887, Val Loss: 1.1557
Epoch 5/50 - Train Loss: 0.8129, Val Loss: 0.7843
Epoch 10/50 - Train Loss: 0.5609, Val Loss: 0.5537
Epoch 15/50 - Train Loss: 0.4527, Val Loss: 0.4576
Epoch 20/50 - Train Loss: 0.4118, Val Loss: 0.4213
Epoch 25/50 - Train Loss: 0.3983, Val Loss: 0.4105
Epoch 30/50 - Train Loss: 0.3947, Val Loss: 0.4078
Epoch 35/50 - Train Loss: 0.3932, Val Loss: 0.4062
Epoch 40/50 - Train Loss: 0.3930, Val Loss: 0.4060
Epoch 45/50 - Train Loss: 0.3922, Val Loss: 0.4062
Epoch 50/50 - Train Loss: 0.3923, Val Loss: 0.4054
```

```
Training model: deep_L5_widths_16_8_8_4_2 (ReLU activation)...
Epoch 1/50 - Train Loss: 1.1013, Val Loss: 1.0626
Epoch 5/50 - Train Loss: 0.8830, Val Loss: 0.8684
Epoch 10/50 - Train Loss: 0.7890, Val Loss: 0.7881
Epoch 15/50 - Train Loss: 0.7645, Val Loss: 0.7672
Epoch 20/50 - Train Loss: 0.7564, Val Loss: 0.7592
Epoch 25/50 - Train Loss: 0.7522, Val Loss: 0.7551
Epoch 30/50 - Train Loss: 0.7493, Val Loss: 0.7531
Epoch 35/50 - Train Loss: 0.7487, Val Loss: 0.7523
Epoch 40/50 - Train Loss: 0.7481, Val Loss: 0.7519
Epoch 45/50 - Train Loss: 0.7478, Val Loss: 0.7517
Epoch 50/50 - Train Loss: 0.7480, Val Loss: 0.7517
```

1.6.5 Evaluation

```
[115]: # --- Plot loss curves for all deep models ---
```

```
for tag, (train_loss, val_loss) in deep_loss_curves.items():
    plt.figure(figsize=(10,6))
    plt.plot(train_loss, label=f'Train Loss - {tag}')
    plt.plot(val_loss, '--', label=f'Val Loss - {tag}')
    plt.xlabel('Epochs')
```

```

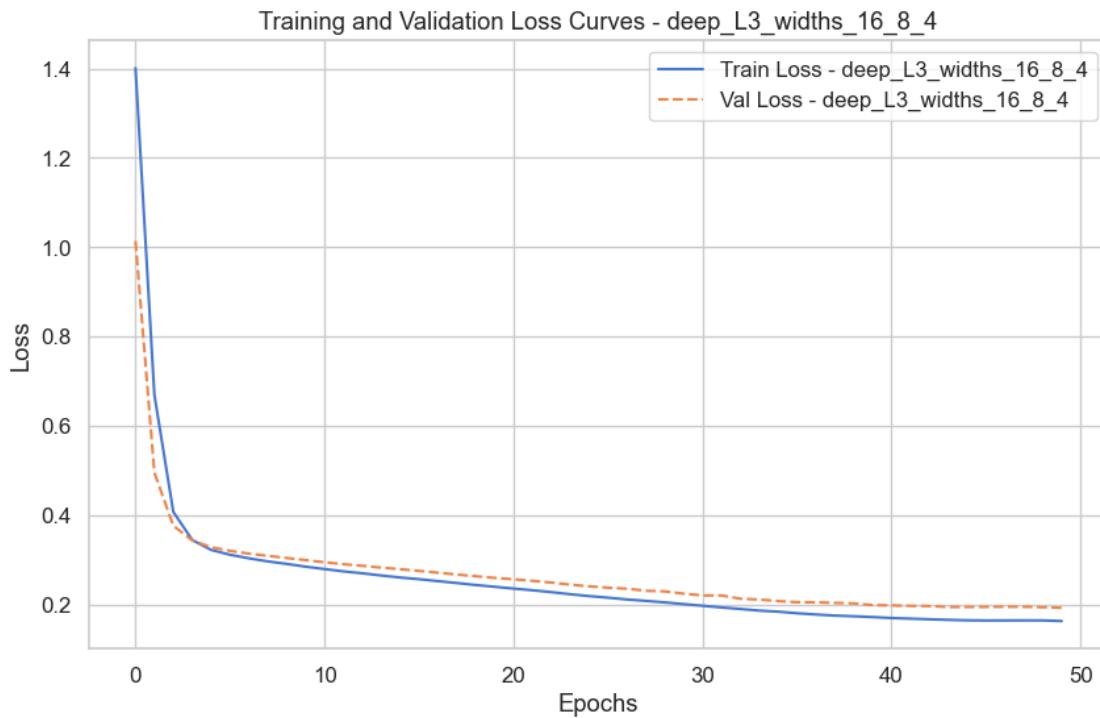
plt.ylabel('Loss')
plt.title(f'Training and Validation Loss Curves - {tag}')
plt.legend()

# Save the plot to the specified path
save_plot(plt.gcf(), f'{tag}_loss_curve', save_dir) # Use plt.gcf() to get the current figure

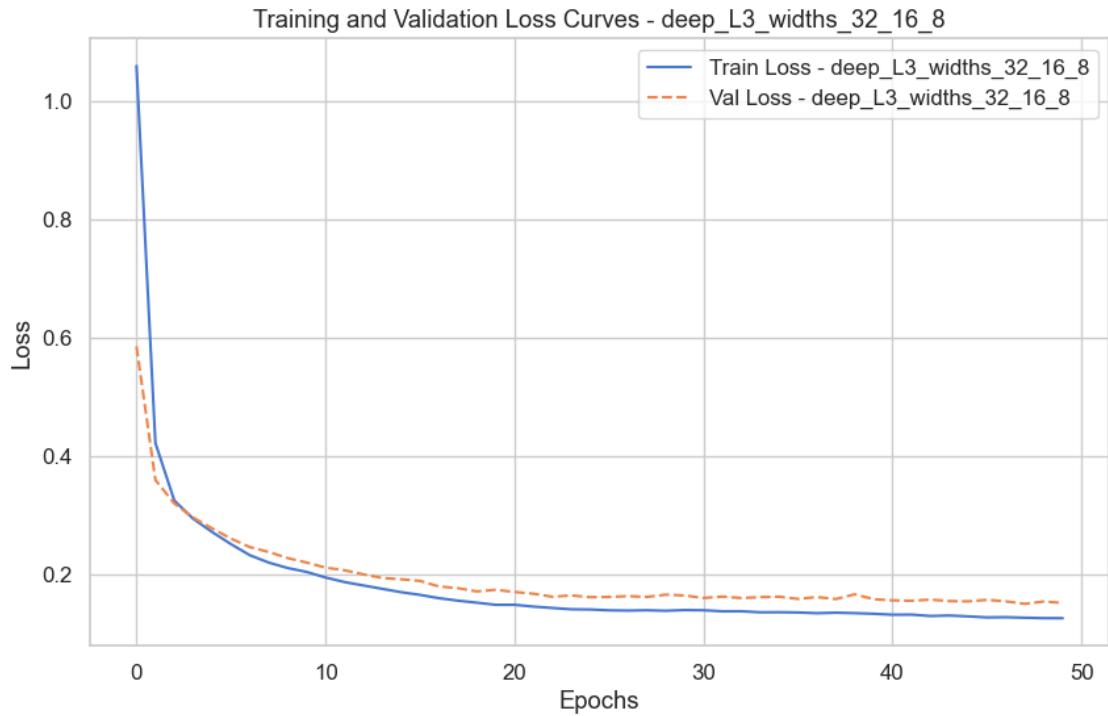
plt.show()

```

Saved plot: ../results/images/task5_plots/deep_L3_widths_16_8_4_loss_curve.png

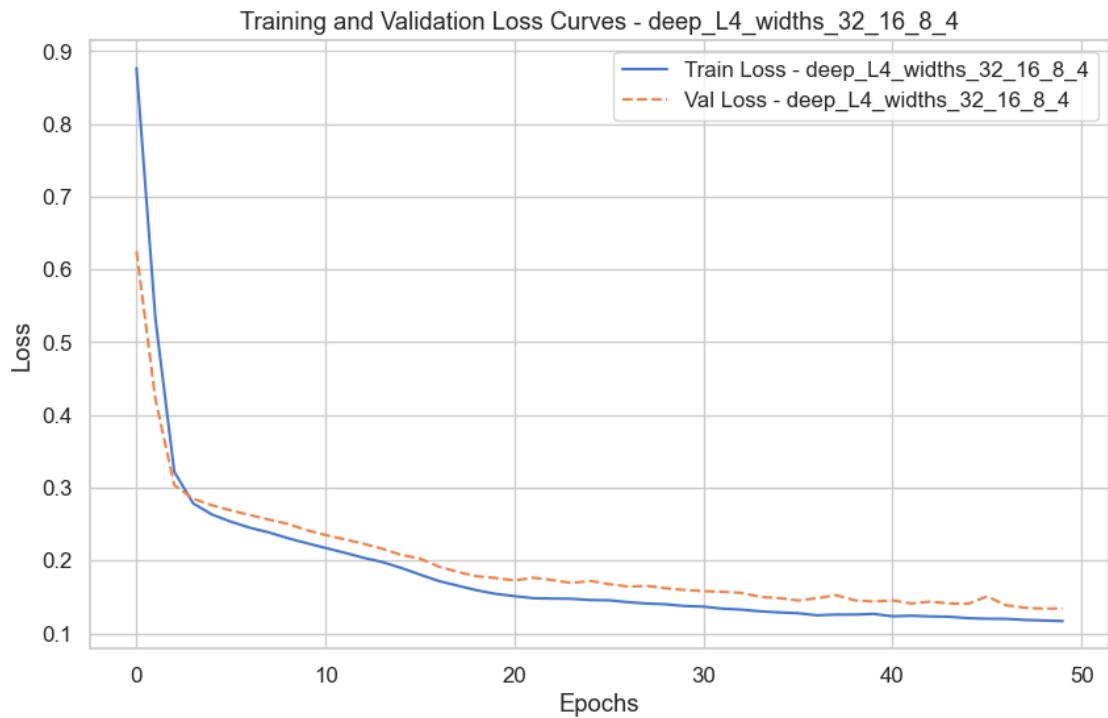


Saved plot: ../results/images/task5_plots/deep_L3_widths_32_16_8_loss_curve.png



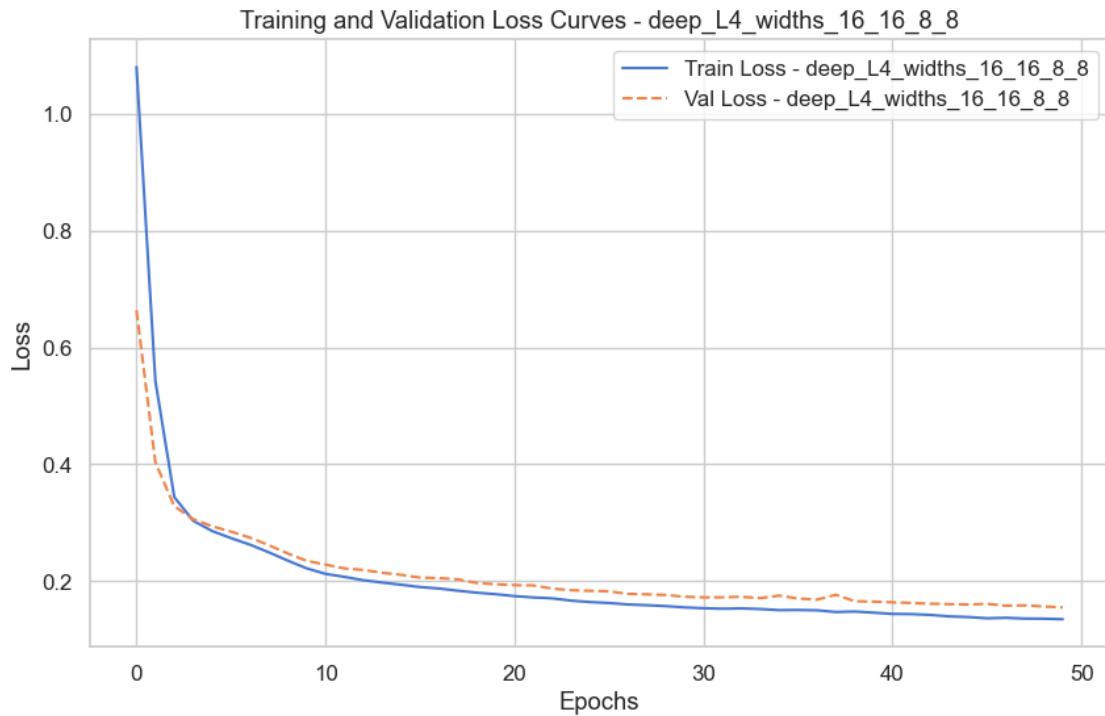
Saved plot:

./results/images/task5_plots/deep_L4_widths_32_16_8_4_loss_curve.png



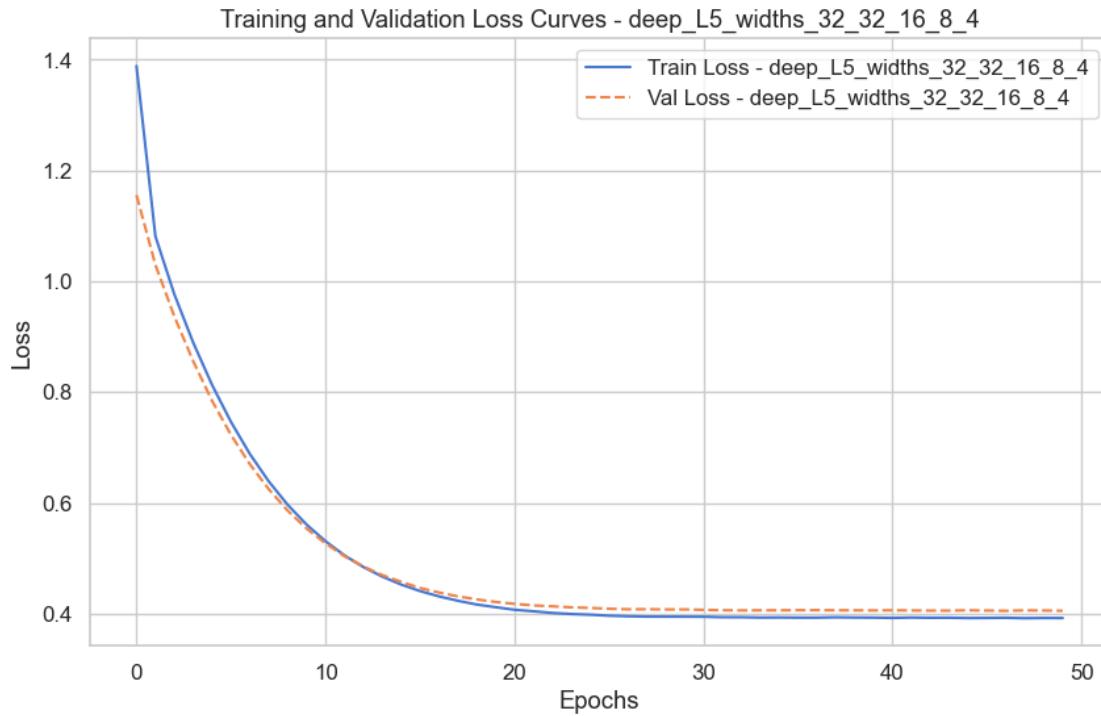
Saved plot:

./results/images/task5_plots/deep_L4_widths_16_16_8_8_loss_curve.png



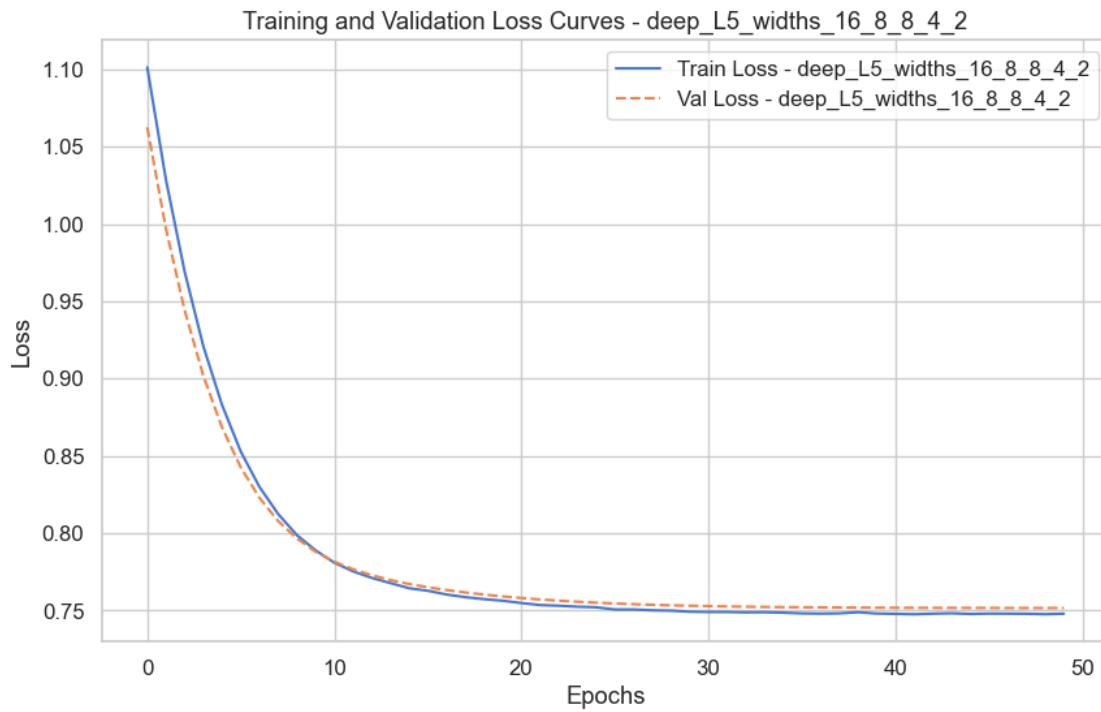
Saved plot:

./results/images/task5_plots/deep_L5_widths_32_32_16_8_4_loss_curve.png



Saved plot:

./results/images/task5_plots/deep_L5_widths_16_8_8_4_2_loss_curve.png



Q: Plot and analyze the losses. Do the models converge? Yes, all models converge properly. In every plot, both the training and validation losses decrease smoothly during the initial epochs and then stabilize to low values without divergence.

```
[116]: # --- Evaluate validation set and identify the best architecture ---  
  
print("\nValidation classification reports for deep models:")  
  
for tag, model in trained_deep_models.items():  
    print(f"\n--- Model {tag} ---")  
  
    # Evaluate on the validation set without the port  
    report = evaluate_model(model, X_val_tensor_no_port, y_val_no_port, tag)  
    print(report)
```

Validation classification reports for deep models:

```
--- Model deep_L3_widths_16_8_4 ---  
      precision    recall   f1-score   support  
  
       0     0.9495    0.9742    0.9617     3378  
       1     0.7975    0.9123    0.8511     285  
       2     0.9752    0.8643    0.9164     774  
       3     0.5000    0.1404    0.2192      57
```

```
      accuracy          0.9408     4494  
macro avg      0.8056    0.7228    0.7371     4494  
weighted avg    0.9386    0.9408    0.9375     4494
```

```
--- Model deep_L3_widths_32_16_8 ---  
      precision    recall   f1-score   support
```

```
       0     0.9530    0.9775    0.9651     3378  
       1     0.8137    0.9193    0.8633     285  
       2     0.9870    0.8824    0.9318     774  
       3     0.2667    0.0702    0.1111      57
```

```
      accuracy          0.9459     4494  
macro avg      0.7551    0.7124    0.7178     4494  
weighted avg    0.9413    0.9459    0.9421     4494
```

```
--- Model deep_L4_widths_32_16_8_4 ---  
      precision    recall   f1-score   support
```

0	0.9596	0.9769	0.9682	3378
1	0.8201	0.9439	0.8777	285
2	0.9696	0.9057	0.9365	774
3	0.5000	0.0351	0.0656	57
accuracy			0.9506	4494
macro avg	0.8123	0.7154	0.7120	4494
weighted avg	0.9466	0.9506	0.9455	4494

--- Model deep_L4_widths_16_16_8_8 ---

	precision	recall	f1-score	support
0	0.9496	0.9819	0.9655	3378
1	0.8359	0.9474	0.8882	285
2	0.9910	0.8540	0.9174	774
3	0.6364	0.1228	0.2059	57
accuracy			0.9468	4494
macro avg	0.8532	0.7265	0.7442	4494
weighted avg	0.9456	0.9468	0.9427	4494

--- Model deep_L5_widths_32_32_16_8_4 ---

Warning: deep_L5_widths_32_32_16_8_4 made no predictions for classes: [1, 3]

	precision	recall	f1-score	support
0	0.8811	1.0000	0.9368	3378
1	0.0000	0.0000	0.0000	285
2	0.9985	0.8514	0.9191	774
3	0.0000	0.0000	0.0000	57
accuracy			0.8983	4494
macro avg	0.4699	0.4629	0.4640	4494
weighted avg	0.8342	0.8983	0.8624	4494

--- Model deep_L5_widths_16_8_8_4_2 ---

Warning: deep_L5_widths_16_8_8_4_2 made no predictions for classes: [1, 2, 3]

	precision	recall	f1-score	support
0	0.7517	1.0000	0.8582	3378
1	0.0000	0.0000	0.0000	285
2	0.0000	0.0000	0.0000	774
3	0.0000	0.0000	0.0000	57
accuracy			0.7517	4494

macro avg	0.1879	0.2500	0.2146	4494
weighted avg	0.5650	0.7517	0.6451	4494

```
[117]: def testing_model(model, dataloader, device):
    """
    Evaluate the model on a given dataloader and compute accuracy.

    Args:
        model: The trained model.
        dataloader: DataLoader for the dataset.
        device: Device to run the model on (CPU or GPU).

    Returns:
        float: Accuracy of the model on the test dataset.
    """
    # Record the start time
    start_time = time.time()

    model.eval()  # Set the model to evaluation mode
    all_labels = []
    all_predictions = []

    with torch.no_grad():  # Disable gradient computation for efficiency
        for inputs, labels in dataloader:
            inputs, labels = inputs.to(device), labels.to(device)  # Move batch to GPU
            outputs = model(inputs)
            _, predicted = torch.max(outputs, 1)  # Get the class with highest score
            all_labels.extend(labels.cpu().numpy())
            all_predictions.extend(predicted.cpu().numpy())

    accuracy = accuracy_score(all_labels, all_predictions) * 100

    # Record the end time
    end_time = time.time()
    # Calculate the elapsed time
    elapsed_time = end_time - start_time
    print(f'The function took {elapsed_time:.4f} seconds to execute.')

    return accuracy
```

```
[118]: for tag, model in trained_deep_models.items():

    print(f'\n--- Model {tag} ---')
    train_accuracy = testing_model(model, train_loader_no_port, "cpu")
```

```

val_accuracy = testing_model(model,val_loader_no_port,"cpu")
test_accuracy = testing_model(model,test_loader_no_port,"cpu")

print(f'Train Accuracy: {train_accuracy:.4f}')
print(f'Validation Accuracy: {val_accuracy:.4f}')
print(f'Test Accuracy: {test_accuracy:.4f}')

```

--- Model deep_L3_widths_16_8_4 ---
The function took 0.0496 seconds to execute.
The function took 0.0152 seconds to execute.
The function took 0.0153 seconds to execute.
Train Accuracy: 94.6072
Validation Accuracy: 94.0810
Test Accuracy: 93.7250

--- Model deep_L3_widths_32_16_8 ---
The function took 0.0457 seconds to execute.
The function took 0.0165 seconds to execute.
The function took 0.0168 seconds to execute.
Train Accuracy: 95.0004
Validation Accuracy: 94.5928
Test Accuracy: 94.4593

--- Model deep_L4_widths_32_16_8_4 ---
The function took 0.0495 seconds to execute.
The function took 0.0154 seconds to execute.
The function took 0.0151 seconds to execute.
Train Accuracy: 95.4603
Validation Accuracy: 95.0601
Test Accuracy: 94.9266

--- Model deep_L4_widths_16_16_8_8 ---
The function took 0.0448 seconds to execute.
The function took 0.0150 seconds to execute.
The function took 0.0150 seconds to execute.
Train Accuracy: 94.8817
Validation Accuracy: 94.6818
Test Accuracy: 94.1923

--- Model deep_L5_widths_32_32_16_8_4 ---
The function took 0.0476 seconds to execute.
The function took 0.0176 seconds to execute.
The function took 0.0155 seconds to execute.
Train Accuracy: 90.1565
Validation Accuracy: 89.8309
Test Accuracy: 89.4971

```

--- Model deep_L5_widths_16_8_8_4_2 ---
The function took 0.0487 seconds to execute.
The function took 0.0162 seconds to execute.
The function took 0.0154 seconds to execute.
Train Accuracy: 75.1650
Validation Accuracy: 75.1669
Test Accuracy: 75.1669

```

Q: Calculate the performance in the validation set and identify the best-performing architecture. How do you select one?

We would like to specify that these values refer to a specific run. They might change if the notebook is processed again.

Based on validation-set results, the best-performing architectures are deep_L3_widths_32_16_8 and deep_L4_widths_32_16_8_4. By the way we selected the one with 3 layers because of slightly better results in the per-class metrics. This model achieves: macro F1 (0.78) and strong accuracy (94.5%). Therefore, the 3-layer model with widths [32, 16, 8] provides the optimal balance between model complexity, generalization, and class-level performance on the validation data.

```
[120]: best_deep_model_tag = 'deep_L3_widths_32_16_8'
model = trained_deep_models[best_deep_model_tag]

print(f"\nTest set classification report ({best_deep_model_tag}):")
report = evaluate_model(model, X_test_tensor_no_port, y_test_no_port)
print(report)
```

Test set classification report (deep_L3_widths_32_16_8):				
	precision	recall	f1-score	support
0	0.9540	0.9751	0.9644	3378
1	0.7964	0.9161	0.8520	286
2	0.9856	0.8836	0.9318	773
3	0.3158	0.1053	0.1579	57
accuracy			0.9446	4494
macro avg	0.7629	0.7200	0.7265	4494
weighted avg	0.9413	0.9446	0.9414	4494

Q: Evaluate and report the performance of the best model in the test set. The test set performance for the best deep model (deep_L3_widths_32_16_8) shows strong overall accuracy (0.94) and weighted F1-score (0.94). The macro average F1-score is also good (0.72), indicating reasonable performance across all classes.

1.6.6 The impact of Batch Size

```
[121]: # --- Experiment with different batch sizes ---

# Assuming 'best_deep_model_tag' and 'trained_deep_models' are available from
# the previous step
best_widths = layer_configs[int(best_deep_model_tag.
    ↪split('_')[1][1])[int(best_deep_model_tag.split('_')[-1].split('_')[0] ==
    ↪str(layer_configs[int(best_deep_model_tag.split('_')[1][1])[0][0]]))]

input_dim_deep = X_train_std_no_port.shape[1]
output_dim_deep = len(np.unique(y_train_no_port))

batch_sizes = [4, 64, 256, 1024]
batch_size_results = {}
batch_size_loss_curves = {}

print(f"\nExperimenting with different batch sizes for the best architecture
    ↪({best_deep_model_tag})...")

for bs in batch_sizes:
    print(f"\nTraining with batch size: {bs}")

    # Create new DataLoaders for the current batch size
    train_loader_bs = DataLoader(TensorDataset(X_train_tensor_no_port,
        ↪y_train_tensor_no_port), batch_size=bs, shuffle=True)
    val_loader_bs = DataLoader(TensorDataset(X_val_tensor_no_port,
        ↪y_val_tensor_no_port), batch_size=bs, shuffle=False)

    # Instantiate a fresh model for each batch size experiment
    model_bs = DeepFFNN(input_dim_deep, best_widths, output_dim_deep,
        ↪activation='relu')

    # Set hyperparameters (same as best ReLU model from Task 2/Task 5 baseline)
    min_delta = 0.00001
    patience = 20
    criterion = nn.CrossEntropyLoss()
    optimizer = optim.AdamW(model_bs.parameters(), lr=0.0005)
    epochs = 50 # Use epochs from deep network training

    # Move model to device
    model_bs = model_bs.to(device)

    start_time = time.time()
    # Training
    model_bs, train_loss_bs, val_loss_bs = train_model(
        model_bs,
```

```

        train_loader_bs,
        val_loader_bs,
        epochs,
        optimizer,
        criterion,
        min_delta,
        patience
    )
end_time = time.time()
training_time = end_time - start_time

model_name = f"deep_L3_widths_{'_'.join(map(str, best_widths))}_bs_{bs}"

# Evaluate on validation set
report_bs = evaluate_model(model_bs, X_val_tensor_no_port, y_val_no_port, model_name)
print(f"\nValidation report for batch size {bs}:")
print(report_bs)

batch_size_results[bs] = {
    'training_time': training_time,
    'validation_report': report_bs
}

batch_size_loss_curves[bs] = (train_loss_bs, val_loss_bs)

# It is now possible to further analyze batch_size_results here, e.g., compare metrics across batch sizes

```

Experimenting with different batch sizes for the best architecture
(deep_L3_widths_32_16_8)...

Training with batch size: 4

Epoch 1/50 - Train Loss: 0.5415, Val Loss: 0.4056
Epoch 5/50 - Train Loss: 0.2150, Val Loss: 0.2231
Epoch 10/50 - Train Loss: 0.1826, Val Loss: 0.2006
Epoch 15/50 - Train Loss: 0.1750, Val Loss: 0.1878
Epoch 20/50 - Train Loss: 0.1550, Val Loss: 0.1664
Epoch 25/50 - Train Loss: 0.1401, Val Loss: 0.1577
Epoch 30/50 - Train Loss: 0.1323, Val Loss: 0.1497
Epoch 35/50 - Train Loss: 0.1297, Val Loss: 0.1550
Epoch 40/50 - Train Loss: 0.1286, Val Loss: 0.1450
Epoch 45/50 - Train Loss: 0.1292, Val Loss: 0.1471
Epoch 50/50 - Train Loss: 0.1268, Val Loss: 0.1374
Warning: deep_L3_widths_16_8_4_bs_4 made no predictions for classes: [3]

Validation report for batch size 4:

	precision	recall	f1-score	support
0	0.9572	0.9739	0.9655	3378
1	0.7947	0.9509	0.8658	285
2	0.9721	0.8992	0.9342	774
3	0.0000	0.0000	0.0000	57
accuracy			0.9473	4494
macro avg	0.6810	0.7060	0.6914	4494
weighted avg	0.9373	0.9473	0.9416	4494

Training with batch size: 64

Epoch 1/50 - Train Loss: 1.3904, Val Loss: 1.2212
 Epoch 5/50 - Train Loss: 0.3335, Val Loss: 0.3226
 Epoch 10/50 - Train Loss: 0.2529, Val Loss: 0.2669
 Epoch 15/50 - Train Loss: 0.2138, Val Loss: 0.2377
 Epoch 20/50 - Train Loss: 0.1837, Val Loss: 0.2068
 Epoch 25/50 - Train Loss: 0.1605, Val Loss: 0.1883
 Epoch 30/50 - Train Loss: 0.1516, Val Loss: 0.1805
 Epoch 35/50 - Train Loss: 0.1424, Val Loss: 0.1716
 Epoch 40/50 - Train Loss: 0.1364, Val Loss: 0.1644
 Epoch 45/50 - Train Loss: 0.1329, Val Loss: 0.1623
 Epoch 50/50 - Train Loss: 0.1300, Val Loss: 0.1593

Warning: deep_L3_widths_16_8_4_bs_64 made no predictions for classes: [3]

Validation report for batch size 64:

	precision	recall	f1-score	support
0	0.9497	0.9790	0.9641	3378
1	0.8154	0.9298	0.8689	285
2	0.9825	0.8721	0.9240	774
3	0.0000	0.0000	0.0000	57
accuracy			0.9450	4494
macro avg	0.6869	0.6952	0.6893	4494
weighted avg	0.9348	0.9450	0.9390	4494

Training with batch size: 256

Epoch 1/50 - Train Loss: 1.3979, Val Loss: 1.3575
 Epoch 5/50 - Train Loss: 0.7072, Val Loss: 0.6695
 Epoch 10/50 - Train Loss: 0.5127, Val Loss: 0.5131
 Epoch 15/50 - Train Loss: 0.4541, Val Loss: 0.4599
 Epoch 20/50 - Train Loss: 0.4160, Val Loss: 0.4265
 Epoch 25/50 - Train Loss: 0.3866, Val Loss: 0.3989
 Epoch 30/50 - Train Loss: 0.3578, Val Loss: 0.3716
 Epoch 35/50 - Train Loss: 0.3306, Val Loss: 0.3469

```
Epoch 40/50 - Train Loss: 0.3069, Val Loss: 0.3235
Epoch 45/50 - Train Loss: 0.2849, Val Loss: 0.3001
Epoch 50/50 - Train Loss: 0.2646, Val Loss: 0.2807
Warning: deep_L3_widths_16_8_4_bs_256 made no predictions for classes: [3]
```

Validation report for batch size 256:

	precision	recall	f1-score	support
0	0.9450	0.9760	0.9602	3378
1	0.7875	0.8842	0.8331	285
2	0.9737	0.8618	0.9143	774
3	0.0000	0.0000	0.0000	57
accuracy			0.9381	4494
macro avg	0.6765	0.6805	0.6769	4494
weighted avg	0.9279	0.9381	0.9321	4494

Training with batch size: 1024

```
Epoch 1/50 - Train Loss: 1.6541, Val Loss: 1.6467
Epoch 5/50 - Train Loss: 1.5940, Val Loss: 1.5855
Epoch 10/50 - Train Loss: 1.4911, Val Loss: 1.4736
Epoch 15/50 - Train Loss: 1.1308, Val Loss: 1.0753
Epoch 20/50 - Train Loss: 0.6396, Val Loss: 0.6101
Epoch 25/50 - Train Loss: 0.4467, Val Loss: 0.4488
Epoch 30/50 - Train Loss: 0.3900, Val Loss: 0.3957
Epoch 35/50 - Train Loss: 0.3538, Val Loss: 0.3643
Epoch 40/50 - Train Loss: 0.3310, Val Loss: 0.3435
Epoch 45/50 - Train Loss: 0.3239, Val Loss: 0.3293
Epoch 50/50 - Train Loss: 0.3061, Val Loss: 0.3198
Warning: deep_L3_widths_16_8_4_bs_1024 made no predictions for classes: [3]
```

Validation report for batch size 1024:

	precision	recall	f1-score	support
0	0.8812	0.9973	0.9357	3378
1	0.0000	0.0000	0.0000	285
2	0.9866	0.8540	0.9155	774
3	0.0000	0.0000	0.0000	57
accuracy			0.8968	4494
macro avg	0.4670	0.4628	0.4628	4494
weighted avg	0.8323	0.8968	0.8610	4494

```
[122]: # --- Plot loss curves for all batch size experiments ---
```

```

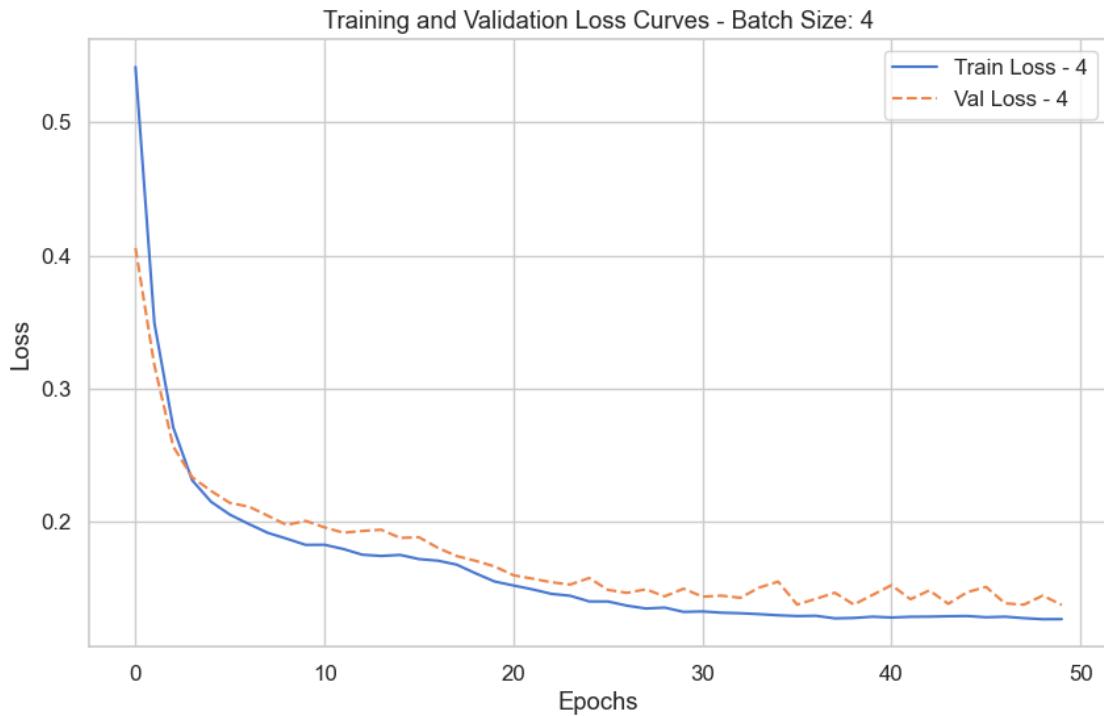
for bs, (train_loss, val_loss) in batch_size_loss_curves.items():
    plt.figure(figsize=(10,6))
    plt.plot(train_loss, label=f'Train Loss - {bs}')
    plt.plot(val_loss, '--', label=f'Val Loss - {bs}')
    plt.xlabel('Epochs')
    plt.ylabel('Loss')
    plt.title(f'Training and Validation Loss Curves - Batch Size: {bs}')
    plt.legend()

    # Save the plot to the specified path
    save_plot(plt.gcf(), f"{bs}_loss_curve", save_dir) # Use plt.gcf() to get the current figure

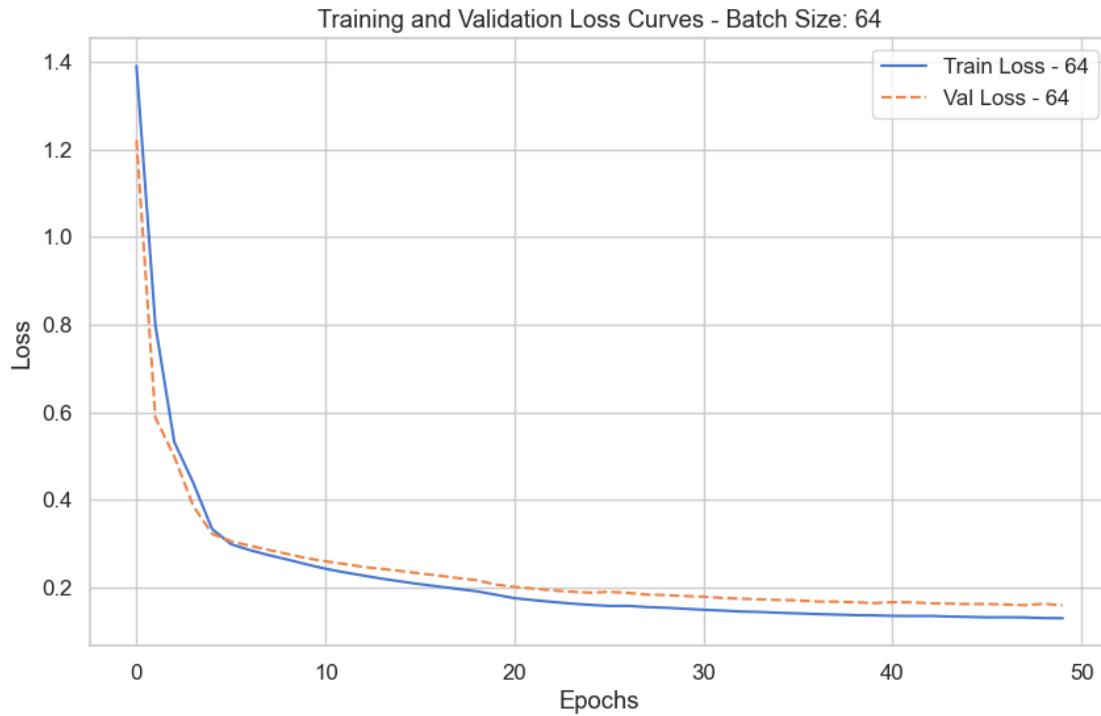
plt.show()

```

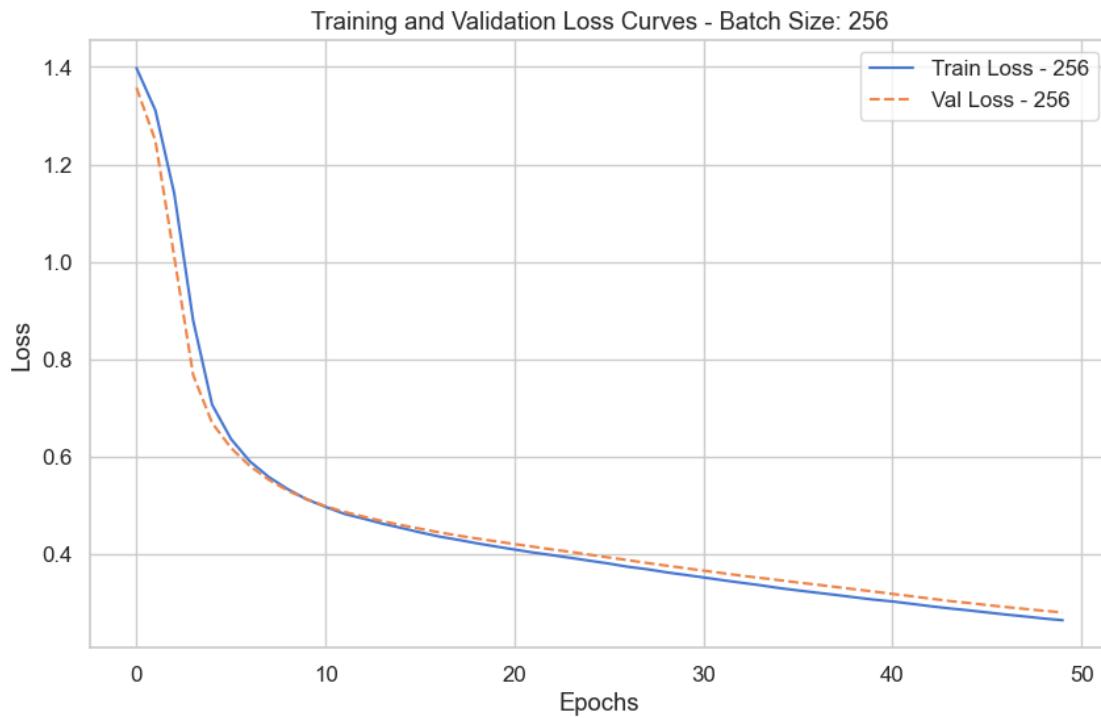
Saved plot: ../results/images/task5_plots/4_loss_curve.png



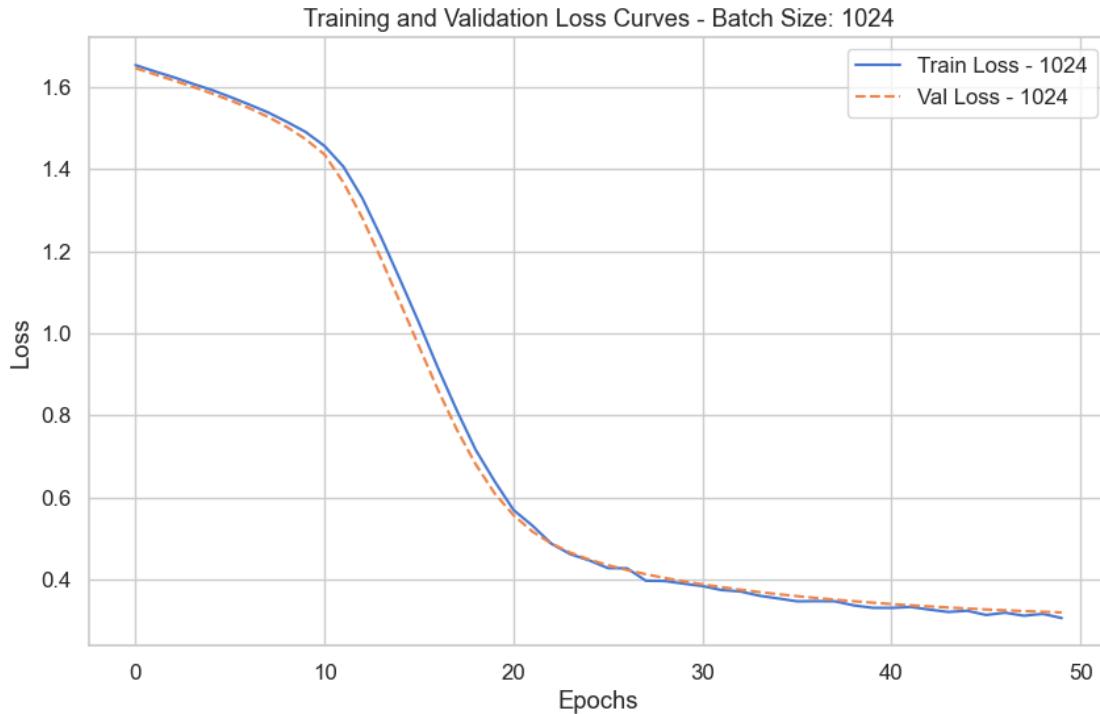
Saved plot: ../results/images/task5_plots/64_loss_curve.png



Saved plot: ./results/images/task5_plots/256_loss_curve.png



Saved plot: ./results/images/task5_plots/1024_loss_curve.png



Q: Use the best hyperparameter identified in the previous step and experiment with different batch sizes. In particular, use as batch size: {4, 64, 256, 1024}. Does performance change? And why? Report the validation results. The batch size strongly affects model performance. Smaller batches (e.g., 4) yield the highest validation accuracy (94.9%) and macro F1 (0.69), while large batches (1024) lead to underfitting and accuracy drops to 89.7%. This occurs because small batches produce noisier gradient updates that enhance generalization, whereas large batches converge to smoother but less optimal minima. Therefore, the model performs best with small or moderate batch sizes (4-64), achieving both stability and high validation performance.

In conclusion, we selected the model with a batch size of 64, as it exhibited the smoothest and most stable loss curve.

```
[123]: # --- Print the times for each batch size training ---

print("\nTraining times for different batch sizes:")
for bs, results in batch_size_results.items():
    print(f"Batch Size {bs}: {results['training_time']:.4f} seconds")
```

Training times for different batch sizes:

Batch Size 4: 55.8748 seconds

Batch Size 64: 5.4656 seconds

```
Batch Size 256: 2.7542 seconds
Batch Size 1024: 3.2436 seconds
```

Q: How long does it take to train the models depending on the batch size? And why?
Training becomes faster with larger batch sizes because the model makes fewer updates per epoch and can process more data at once, using the hardware more efficiently.

That's why the jump from batch size 4 → 64 → 256 greatly reduces training time.

However, going from 256 to 1024 gives only a small speed gain — the hardware is already fully used, so the improvement levels off.

1.6.7 The impact of the Optimizer

```
[128]: # --- Experiment with different optimizers ---

# Assuming 'best_deep_model_tag' and 'best_widths' are available
input_dim_deep = X_train_std_no_port.shape[1]
output_dim_deep = len(np.unique(y_train_no_port))
batch_size_opt = 64 # Use a reasonable batch size, e.g., 64

# Create DataLoaders for optimizer experiments
train_loader_opt = DataLoader(TensorDataset(X_train_tensor_no_port, ▾
    ↵y_train_tensor_no_port), batch_size=batch_size_opt, shuffle=True)
val_loader_opt = DataLoader(TensorDataset(X_val_tensor_no_port, ▾
    ↵y_val_tensor_no_port), batch_size=batch_size_opt, shuffle=False)

optimizers_to_test = {
    'SGD': optim.SGD,
    'SGD_momentum_0.1': lambda params, lr: optim.SGD(params, lr=lr, momentum=0.
    ↵1),
    'SGD_momentum_0.5': lambda params, lr: optim.SGD(params, lr=lr, momentum=0.
    ↵5),
    'SGD_momentum_0.9': lambda params, lr: optim.SGD(params, lr=lr, momentum=0.
    ↵9),
    'AdamW': optim.AdamW
}

optimizer_results = {}
optimizer_loss_curves = {}
trained_opt_models = {}

print(f"\nExperimenting with different optimizers for the best architecture_"
    ↵({best_deep_model_tag})...")

for opt_name, opt_class in optimizers_to_test.items():
    print(f"\nTraining with optimizer: {opt_name}":
```

```

# Instantiate a fresh model for each optimizer experiment
model_opt = DeepFFNN(input_dim_deep, best_widths, output_dim_deep, □
activation='relu')

# Set hyperparameters (same as best ReLU model from Task 2/Task 5 baseline, □
but with optimizer variations)
min_delta = 0.00001
patience = 20
criterion = nn.CrossEntropyLoss()
lr = 0.0005 # Initial learning rate
epochs = 50 # Use epochs from deep network training

# Instantiate the optimizer
if opt_name in ['SGD', 'AdamW']:
    optimizer = opt_class(model_opt.parameters(), lr=lr)
else:
    optimizer = opt_class(model_opt.parameters(), lr=lr)

# Move model to device
model_opt = model_opt.to(device)

start_time = time.time()
# Training
model_opt, train_loss_opt, val_loss_opt = train_model(
    model_opt,
    train_loader_opt,
    val_loader_opt,
    epochs,
    optimizer,
    criterion,
    min_delta,
    patience
)
end_time = time.time()
training_time = end_time - start_time

trained_opt_models[opt_name] = model_opt

model_name = f"deep_L3_widths_{'_'.join(map(str, □
best_widths))}_{opt_name}""

# Evaluate on validation set
report_opt = evaluate_model(model_opt, X_val_tensor_no_port, y_val_no_port, □
model_name)
print(f"\nValidation report for optimizer {opt_name}:")
print(report_opt)

```

```

optimizer_results[opt_name] = {
    'training_time': training_time,
    'validation_report': report_opt
}

optimizer_loss_curves[opt_name] = (train_loss_opt, val_loss_opt)

```

Experimenting with different optimizers for the best architecture
(deep_L3_widths_32_16_8)...

Training with optimizer: SGD

Epoch 1/50 - Train Loss: 1.5335, Val Loss: 1.5106
Epoch 5/50 - Train Loss: 1.3680, Val Loss: 1.3500
Epoch 10/50 - Train Loss: 1.2039, Val Loss: 1.1913
Epoch 15/50 - Train Loss: 1.0805, Val Loss: 1.0725
Epoch 20/50 - Train Loss: 0.9898, Val Loss: 0.9853
Epoch 25/50 - Train Loss: 0.9232, Val Loss: 0.9213
Epoch 30/50 - Train Loss: 0.8733, Val Loss: 0.8734
Epoch 35/50 - Train Loss: 0.8339, Val Loss: 0.8355
Epoch 40/50 - Train Loss: 0.8002, Val Loss: 0.8029
Epoch 45/50 - Train Loss: 0.7678, Val Loss: 0.7708
Epoch 50/50 - Train Loss: 0.7311, Val Loss: 0.7344
Warning: deep_L3_widths_16_8_4_opt_SGD made no predictions for classes: [1, 3]

Validation report for optimizer SGD:

	precision	recall	f1-score	support
0	0.7514	0.9985	0.8575	3378
1	0.0000	0.0000	0.0000	285
2	0.0000	0.0000	0.0000	774
3	0.0000	0.0000	0.0000	57
accuracy			0.7506	4494
macro avg	0.1878	0.2496	0.2144	4494
weighted avg	0.5648	0.7506	0.6446	4494

Training with optimizer: SGD_momentum_0.1

Epoch 1/50 - Train Loss: 1.2371, Val Loss: 1.2194
Epoch 5/50 - Train Loss: 1.1096, Val Loss: 1.0967
Epoch 10/50 - Train Loss: 0.9937, Val Loss: 0.9859
Epoch 15/50 - Train Loss: 0.9150, Val Loss: 0.9110
Epoch 20/50 - Train Loss: 0.8624, Val Loss: 0.8609
Epoch 25/50 - Train Loss: 0.8274, Val Loss: 0.8276
Epoch 30/50 - Train Loss: 0.8036, Val Loss: 0.8052
Epoch 35/50 - Train Loss: 0.7870, Val Loss: 0.7896
Epoch 40/50 - Train Loss: 0.7751, Val Loss: 0.7780

```
Epoch 45/50 - Train Loss: 0.7653, Val Loss: 0.7683
Epoch 50/50 - Train Loss: 0.7560, Val Loss: 0.7592
Warning: deep_L3_widths_16_8_4_opt_SGD_momentum_0.1 made no predictions for
classes: [1, 2, 3]
```

```
Validation report for optimizer SGD_momentum_0.1:
      precision    recall  f1-score   support

          0       0.7517    1.0000    0.8582      3378
          1       0.0000    0.0000    0.0000      285
          2       0.0000    0.0000    0.0000      774
          3       0.0000    0.0000    0.0000       57

   accuracy                           0.7517      4494
  macro avg       0.1879    0.2500    0.2146      4494
weighted avg     0.5650    0.7517    0.6451      4494
```

```
Training with optimizer: SGD_momentum_0.5
Epoch 1/50 - Train Loss: 1.2908, Val Loss: 1.2541
Epoch 5/50 - Train Loss: 1.0555, Val Loss: 1.0328
Epoch 10/50 - Train Loss: 0.8835, Val Loss: 0.8729
Epoch 15/50 - Train Loss: 0.7981, Val Loss: 0.7945
Epoch 20/50 - Train Loss: 0.7563, Val Loss: 0.7565
Epoch 25/50 - Train Loss: 0.7325, Val Loss: 0.7341
Epoch 30/50 - Train Loss: 0.7138, Val Loss: 0.7165
Epoch 35/50 - Train Loss: 0.6941, Val Loss: 0.6960
Epoch 40/50 - Train Loss: 0.6640, Val Loss: 0.6665
Epoch 45/50 - Train Loss: 0.6316, Val Loss: 0.6354
Epoch 50/50 - Train Loss: 0.6095, Val Loss: 0.6144
Warning: deep_L3_widths_16_8_4_opt_SGD_momentum_0.5 made no predictions for
classes: [1, 2, 3]
```

```
Validation report for optimizer SGD_momentum_0.5:
      precision    recall  f1-score   support

          0       0.7517    1.0000    0.8582      3378
          1       0.0000    0.0000    0.0000      285
          2       0.0000    0.0000    0.0000      774
          3       0.0000    0.0000    0.0000       57

   accuracy                           0.7517      4494
  macro avg       0.1879    0.2500    0.2146      4494
weighted avg     0.5650    0.7517    0.6451      4494
```

```
Training with optimizer: SGD_momentum_0.9
Epoch 1/50 - Train Loss: 1.4210, Val Loss: 1.2344
```

Epoch 5/50 - Train Loss: 0.8057, Val Loss: 0.7870
 Epoch 10/50 - Train Loss: 0.5710, Val Loss: 0.5421
 Epoch 15/50 - Train Loss: 0.3828, Val Loss: 0.3893
 Epoch 20/50 - Train Loss: 0.3547, Val Loss: 0.3638
 Epoch 25/50 - Train Loss: 0.3366, Val Loss: 0.3460
 Epoch 30/50 - Train Loss: 0.3199, Val Loss: 0.3300
 Epoch 35/50 - Train Loss: 0.3028, Val Loss: 0.3133
 Epoch 40/50 - Train Loss: 0.2887, Val Loss: 0.3012
 Epoch 45/50 - Train Loss: 0.2790, Val Loss: 0.2929
 Epoch 50/50 - Train Loss: 0.2708, Val Loss: 0.2870
 Warning: deep_L3_widths_16_8_4_opt_SGD_momentum_0.9 made no predictions for classes: [3]

Validation report for optimizer SGD_momentum_0.9:

	precision	recall	f1-score	support
0	0.8811	0.9979	0.9359	3378
1	0.0000	0.0000	0.0000	285
2	0.9880	0.8514	0.9146	774
3	0.0000	0.0000	0.0000	57
accuracy			0.8968	4494
macro avg	0.4673	0.4623	0.4626	4494
weighted avg	0.8324	0.8968	0.8610	4494

Training with optimizer: AdamW

Epoch 1/50 - Train Loss: 1.6180, Val Loss: 1.4255
 Epoch 5/50 - Train Loss: 0.3073, Val Loss: 0.3058
 Epoch 10/50 - Train Loss: 0.2515, Val Loss: 0.2646
 Epoch 15/50 - Train Loss: 0.2275, Val Loss: 0.2470
 Epoch 20/50 - Train Loss: 0.2092, Val Loss: 0.2332
 Epoch 25/50 - Train Loss: 0.1925, Val Loss: 0.2179
 Epoch 30/50 - Train Loss: 0.1803, Val Loss: 0.2094
 Epoch 35/50 - Train Loss: 0.1728, Val Loss: 0.2037
 Epoch 40/50 - Train Loss: 0.1690, Val Loss: 0.1970
 Epoch 45/50 - Train Loss: 0.1659, Val Loss: 0.1955
 Epoch 50/50 - Train Loss: 0.1664, Val Loss: 0.1961

Validation report for optimizer AdamW:

	precision	recall	f1-score	support
0	0.9484	0.9731	0.9605	3378
1	0.7844	0.8807	0.8298	285
2	0.9824	0.8643	0.9196	774
3	0.4815	0.2281	0.3095	57
accuracy			0.9390	4494

macro avg	0.7991	0.7365	0.7549	4494
weighted avg	0.9379	0.9390	0.9369	4494

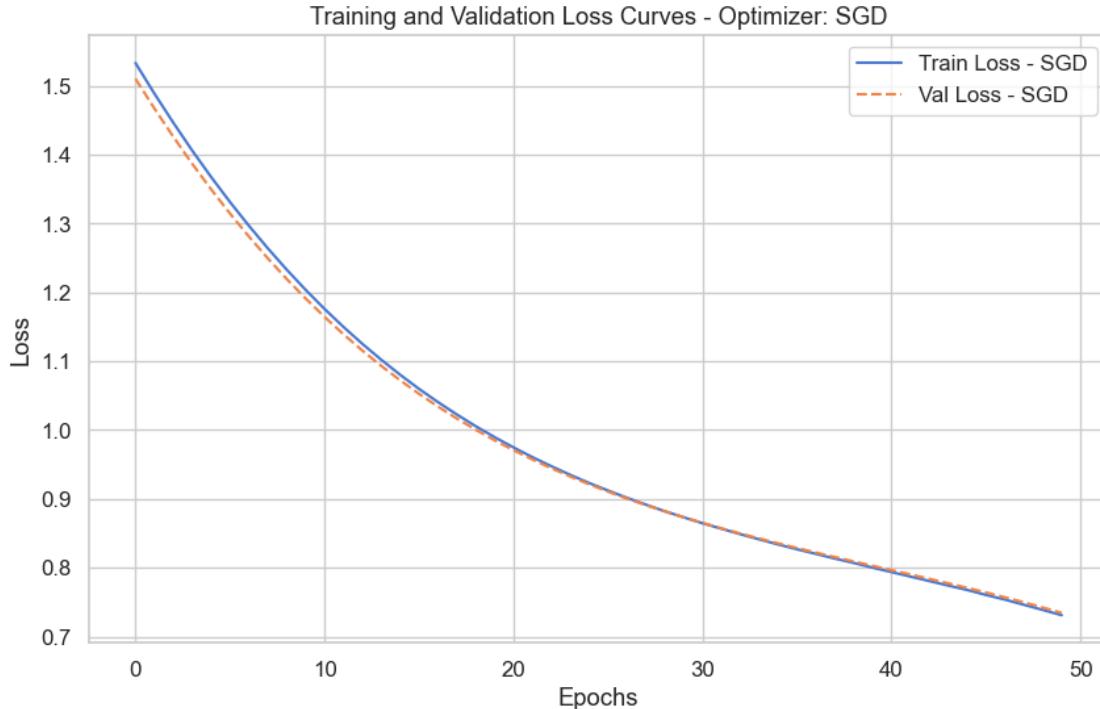
```
[129]: # --- Plot loss curves for all optimizer experiments ---

for opt_name, (train_loss, val_loss) in optimizer_loss_curves.items():
    plt.figure(figsize=(10,6))
    plt.plot(train_loss, label=f'Train Loss - {opt_name}')
    plt.plot(val_loss, '--', label=f'Val Loss - {opt_name}')
    plt.xlabel('Epochs')
    plt.ylabel('Loss')
    plt.title(f'Training and Validation Loss Curves - Optimizer: {opt_name}')
    plt.legend()

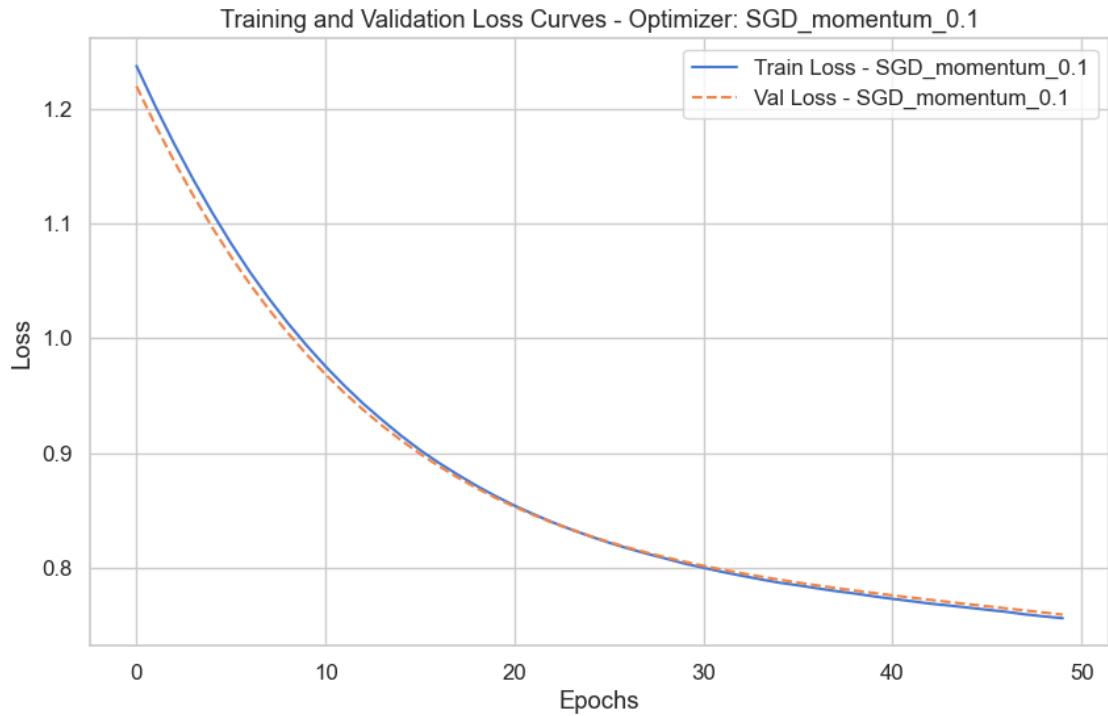
    # Save the plot to the specified path
    save_plot(plt.gcf(), f"{opt_name}_loss_curve", save_dir) # Use plt.gcf() to
    # get the current figure

plt.show()
```

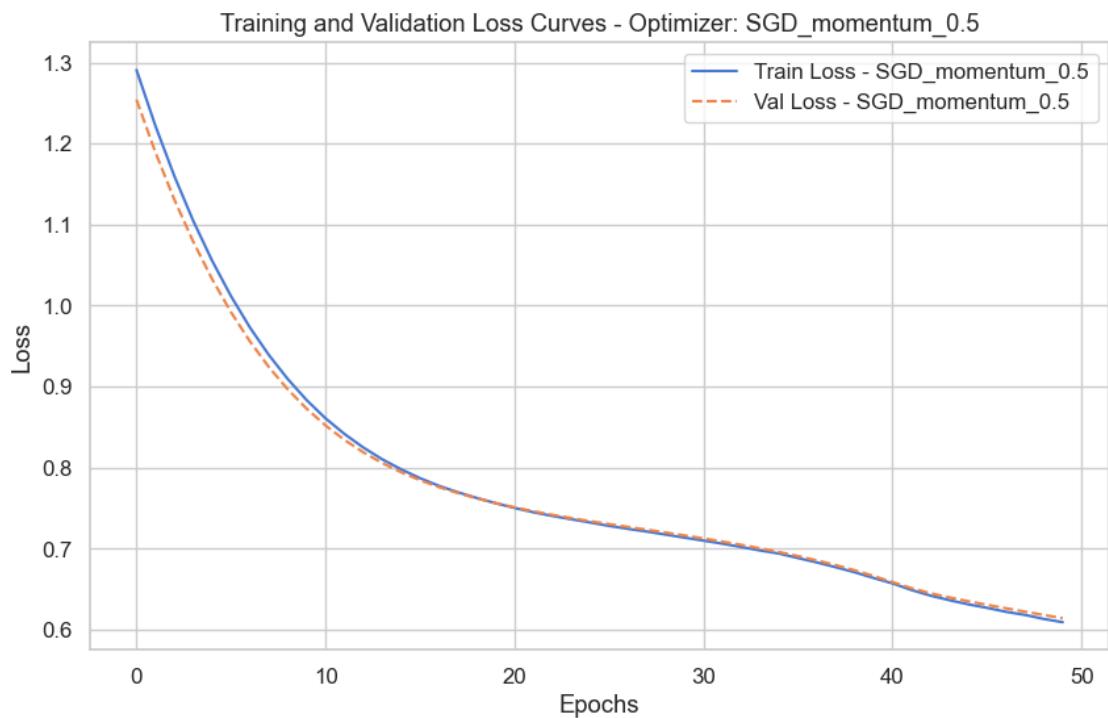
Saved plot: ../results/images/task5_plots/SGD_loss_curve.png



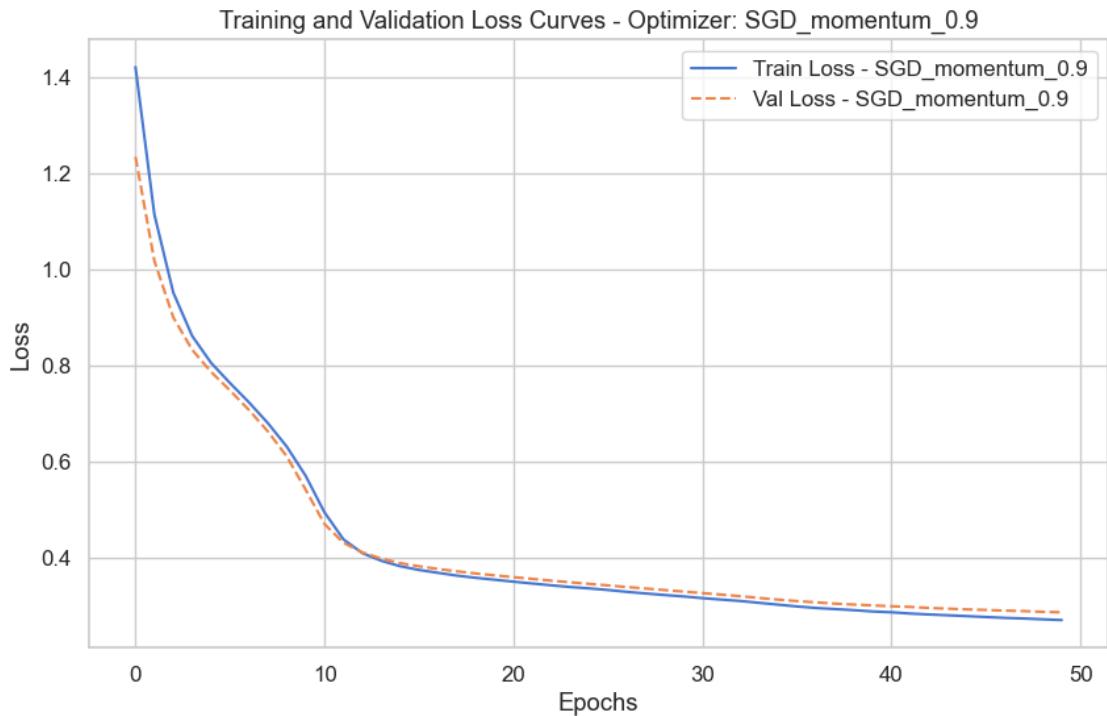
Saved plot: ../results/images/task5_plots/SGD_momentum_0.1_loss_curve.png



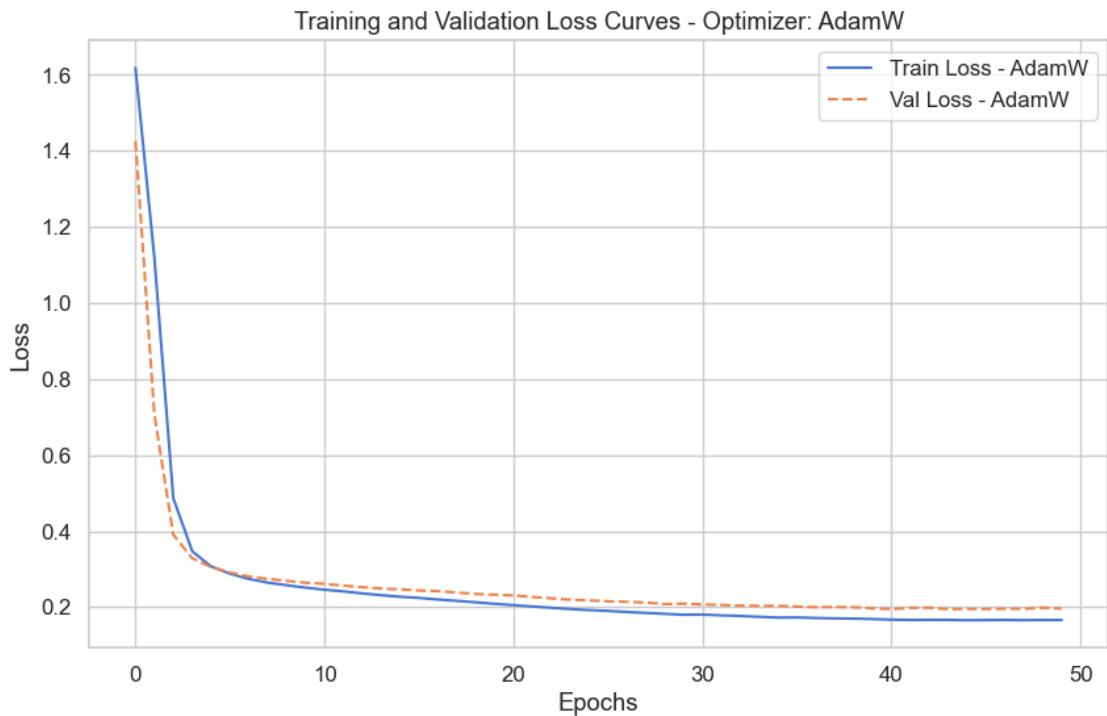
Saved plot: ./results/images/task5_plots/SGD_momentum_0.5_loss_curve.png



Saved plot: ./results/images/task5_plots/SGD_momentum_0.9_loss_curve.png



Saved plot: ./results/images/task5_plots/AdamW_loss_curve.png



Q: Finally, evaluate here how the optimizers affect the classification performance, training time and loss trend. The evaluated optimizers are: Stochastic Gradient Descent (SGD), SGD with Momentum(0.1, 0.5, 0.9) and AdamW. Is there a difference in the trend of the loss functions? Yes, there is a clear difference in the loss trends:

- **AdamW** converges much faster and reaches a lower loss for both training and validation, showing efficient optimization and stable learning.
- **SGD without momentum** converges very slowly, with both losses staying high.
- **SGD with momentum** improves convergence as momentum increases ($0.1 \rightarrow 0.9$), but still remains slower and less effective than AdamW.

In summary, **AdamW** shows the steepest and smoothest loss decrease, while SGD variants converge gradually, with higher final losses.

```
[130]: # --- Print the times for each batch size training ---
```

```
print("\nTraining times for different optimizers:")
for opt_name, results in optimizer_results.items():
    print(f"Optimizer {opt_name}: {results['training_time']:.4f} seconds")
```

```
Training times for different optimizers:
Optimizer SGD: 5.3055 seconds
Optimizer SGD_momentum_0.1: 4.5329 seconds
Optimizer SGD_momentum_0.5: 4.5588 seconds
Optimizer SGD_momentum_0.9: 4.5429 seconds
Optimizer AdamW: 5.5439 seconds
```

Q: How long does it take to train the models with the different optimizers? And why?
All runs use the same 50 epochs, so time mainly reflects per-update compute:

- **SGD with momentum** was fastest (4.5 s) because momentum smooths gradient updates, improving efficiency.
- **Plain SGD** (5.3 s) was slower due to noisier updates, and **AdamW** (5.5 s) took slightly longer because its adaptive learning-rate and weight-decay computations add overhead.

Q: Now, focus on the architecture with the best optimizer. Evaluate the effects of the different learning rates and epochs. Report the test results for the best model.

```
[131]: best_opt_model_tag = 'AdamW'
model = trained_opt_models[best_opt_model_tag]

print(f"\nTest set classification report ({best_opt_model_tag}):")
report = evaluate_model(model, X_test_tensor_no_port, y_test_no_port)
print(report)
```

```

Test set classification report (AdamW):
    precision    recall   f1-score   support

      0       0.9460    0.9701    0.9579     3378
      1       0.7625    0.9091    0.8293      286
      2       0.9835    0.8461    0.9096     773
      3       0.5000    0.2105    0.2963      57

  accuracy                           0.9352    4494
macro avg       0.7980    0.7339    0.7483    4494
weighted avg    0.9351    0.9352    0.9330    4494

```

1.7 Task 6 — Overfitting and Regularization

We analyze overfitting and apply regularization techniques to improve generalization.

Base model: - Layers: **6** - Hidden widths: [256, 128, 64, 32, 16] - Activation: **ReLU** - Optimizer: **AdamW**, learning rate = 5e-4 - Batch size: **128** - Epochs: up to 50

Steps: - Train baseline model and inspect loss curves for overfitting. - Add **Dropout**, **Batch Normalization**, and **Weight Decay** (AdamW regularization). - Compare validation/test performance across variants. - Discuss which regularization technique best mitigates overfitting.

```
[132]: # Create directory for plots
save_dir = results_path + 'images/' + 'task6_plots/'
os.makedirs(save_dir, exist_ok=True)
```

1.7.1 Training

```
[133]: # --- Define 6-layer FFNN with Regularization Options ---

class RegularizedDeepFFNN(nn.Module):
    def __init__(self, input_dim, layer_widths, output_dim, activation='relu', ↴
                 dropout_prob=0.0, use_batchnorm=False):
        super(RegularizedDeepFFNN, self).__init__()
        layers = []
        prev_width = input_dim
        for i, width in enumerate(layer_widths):
            layers.append(nn.Linear(prev_width, width))
            if use_batchnorm:
                layers.append(nn.BatchNorm1d(width))
            if activation == 'relu':
                layers.append(nn.ReLU())
            if dropout_prob > 0 and i < len(layer_widths) - 1: # Apply dropout ↴
                to hidden layers
                layers.append(nn.Dropout(dropout_prob))
        prev_width = width
```

```
    layers.append(nn.Linear(prev_width, output_dim))
    self.net = nn.Sequential(*layers)
```

```
def forward(self, x):
    return self.net(x)
```

[134]: # --- Experiment with Regularization ---

```
input_dim_reg = X_train_std_no_port.shape[1]
output_dim_reg = len(np.unique(y_train_no_port))
layer_widths_reg = [256, 128, 64, 32, 16] # Same widths as the baseline 6-layer model

# Define hyperparameters for regularization experiments
base_lr = 0.0005
epochs_reg = 50
batch_size_reg = 128
min_delta_reg = 0.00001
patience_reg = 20

regularization_configs = {
    'Baseline': # No dropout, no batch norm, no weight decay
        {'dropout_prob': 0.0, 'use_batchnorm': False, 'weight_decay': 0.0},
    'Dropout_0.5': # Dropout 50% (no BN, no weight decay)
        {'dropout_prob': 0.5, 'use_batchnorm': False, 'weight_decay': 0.0},
    'BatchNorm': # Batch normalization only
        {'use_batchnorm': True, 'dropout_prob': 0.0, 'weight_decay': 0.0},
    'BatchNorm_Dropout_0.5': # BatchNorm + Dropout 50%
        {'use_batchnorm': True, 'dropout_prob': 0.5, 'weight_decay': 0.0},
    'WeightDecay_1e-4': # L2 regularization via weight_decay=1e-4 (no dropout, no BN)
        {'dropout_prob': 0.0, 'use_batchnorm': False, 'weight_decay': 1e-4},
    'WeightDecay_1e-4_BN_Dropout_0.5': # All three: BatchNorm + Dropout 50% + Weight Decay 1e-4
        {'use_batchnorm': True, 'dropout_prob': 0.5, 'weight_decay': 1e-4}
}

regularized_models = {}
regularized_loss_curves = {}
regularized_validation_reports = {}
regularized_test_reports = {}

for config_name, params in regularization_configs.items():
    print(f"\nTraining model with {config_name}...")

    # Instantiate model with regularization
    model_reg = RegularizedDeepFFNN(
```

```

        input_dim_reg,
        layer_widths_reg,
        output_dim_reg,
        activation='relu',
        dropout_prob=params.get('dropout_prob', 0.0),
        use_batchnorm=params.get('use_batchnorm', False)
    )

# Define optimizer with weight decay
optimizer_reg = optim.AdamW(model_reg.parameters(), lr=base_lr,
                           weight_decay=params.get('weight_decay', 0.0))
criterion = nn.CrossEntropyLoss()

# Create DataLoaders (using the same as the baseline 6-layer model)
train_loader_reg = train_loader_no_port
val_loader_reg = val_loader_no_port

# Move model to device
model_reg = model_reg.to(device)

# Training
model_reg, train_loss_reg, val_loss_reg = train_model(
    model_reg,
    train_loader_reg,
    val_loader_reg,
    epochs_reg,
    optimizer_reg,
    criterion,
    min_delta=min_delta_reg,
    patience=patience_reg
)

regularized_models[config_name] = model_reg
regularized_loss_curves[config_name] = (train_loss_reg, val_loss_reg)

model_name = f"deep_L3_widths_{'_'.join(map(str,
layer_widths_reg))}_{config_name}""

# Evaluate on validation set
report_val_reg = evaluate_model(model_reg, X_val_tensor_no_port,
                                 y_val_no_port, model_name)
regularized_validation_reports[config_name] = report_val_reg
print(f"\nValidation report for {config_name}:")
print(report_val_reg)

# Evaluate on test set

```

```

    report_test_reg = evaluate_model(model_reg, X_test_tensor_no_port, y_test_no_port)
    regularized_test_reports[config_name] = report_test_reg
    print(f"\nTest report for {config_name}:")
    print(report_test_reg)

# It is now possible compare the reports in regularized_validation_reports and
# regularized_test_reports

```

Training model with Baseline...

```

Epoch 1/50 - Train Loss: 0.5173, Val Loss: 0.3061
Epoch 5/50 - Train Loss: 0.1596, Val Loss: 0.1743
Epoch 10/50 - Train Loss: 0.1285, Val Loss: 0.1380
Epoch 15/50 - Train Loss: 0.1228, Val Loss: 0.1478
Epoch 20/50 - Train Loss: 0.1155, Val Loss: 0.1316
Epoch 25/50 - Train Loss: 0.1120, Val Loss: 0.1249
Epoch 30/50 - Train Loss: 0.1099, Val Loss: 0.1217
Epoch 35/50 - Train Loss: 0.1036, Val Loss: 0.1207
Epoch 40/50 - Train Loss: 0.1050, Val Loss: 0.1286
Epoch 45/50 - Train Loss: 0.1015, Val Loss: 0.1306
Epoch 50/50 - Train Loss: 0.1016, Val Loss: 0.1225

```

Validation report for Baseline:

	precision	recall	f1-score	support
0	0.9585	0.9908	0.9744	3378
1	0.9308	0.9439	0.9373	285
2	0.9872	0.8953	0.9390	774
3	0.3636	0.0702	0.1176	57
accuracy			0.9597	4494
macro avg	0.8100	0.7251	0.7421	4494
weighted avg	0.9541	0.9597	0.9551	4494

Test report for Baseline:

	precision	recall	f1-score	support
0	0.9601	0.9899	0.9748	3378
1	0.9249	0.9476	0.9361	286
2	0.9872	0.8991	0.9411	773
3	0.2857	0.0702	0.1127	57
accuracy			0.9599	4494
macro avg	0.7895	0.7267	0.7412	4494
weighted avg	0.9540	0.9599	0.9556	4494

Training model with Dropout_0.5...

Epoch 1/50 - Train Loss: 0.6897, Val Loss: 0.3460
 Epoch 5/50 - Train Loss: 0.2761, Val Loss: 0.2574
 Epoch 10/50 - Train Loss: 0.1977, Val Loss: 0.1868
 Epoch 15/50 - Train Loss: 0.1774, Val Loss: 0.1641
 Epoch 20/50 - Train Loss: 0.1671, Val Loss: 0.1558
 Epoch 25/50 - Train Loss: 0.1568, Val Loss: 0.1460
 Epoch 30/50 - Train Loss: 0.1500, Val Loss: 0.1435
 Epoch 35/50 - Train Loss: 0.1493, Val Loss: 0.1415
 Epoch 40/50 - Train Loss: 0.1489, Val Loss: 0.1439
 Epoch 45/50 - Train Loss: 0.1436, Val Loss: 0.1380
 Epoch 50/50 - Train Loss: 0.1405, Val Loss: 0.1350
 Warning: deep_L3_widths_256_128_64_32_16_reg_Dropout_0.5 made no predictions for classes: [3]

Validation report for Dropout_0.5:

	precision	recall	f1-score	support
0	0.9490	0.9796	0.9640	3378
1	0.8133	0.9474	0.8752	285
2	0.9881	0.8618	0.9206	774
3	0.0000	0.0000	0.0000	57
accuracy			0.9448	4494
macro avg	0.6876	0.6972	0.6900	4494
weighted avg	0.9351	0.9448	0.9387	4494

Warning: Unnamed model made no predictions for classes: [3]

Test report for Dropout_0.5:

	precision	recall	f1-score	support
0	0.9459	0.9775	0.9614	3378
1	0.7953	0.9510	0.8662	286
2	0.9909	0.8473	0.9135	773
3	0.0000	0.0000	0.0000	57
accuracy			0.9410	4494
macro avg	0.6830	0.6940	0.6853	4494
weighted avg	0.9320	0.9410	0.9349	4494

Training model with BatchNorm...

Epoch 1/50 - Train Loss: 0.7893, Val Loss: 0.4539
 Epoch 5/50 - Train Loss: 0.1633, Val Loss: 0.1759
 Epoch 10/50 - Train Loss: 0.1427, Val Loss: 0.2133
 Epoch 15/50 - Train Loss: 0.1406, Val Loss: 0.1709

Epoch 20/50 - Train Loss: 0.1403, Val Loss: 0.1505
Epoch 25/50 - Train Loss: 0.1332, Val Loss: 0.1583
Epoch 30/50 - Train Loss: 0.1308, Val Loss: 0.1483
Epoch 35/50 - Train Loss: 0.1191, Val Loss: 0.2144
Epoch 40/50 - Train Loss: 0.1186, Val Loss: 0.1744
Epoch 45/50 - Train Loss: 0.1247, Val Loss: 0.1237
Epoch 50/50 - Train Loss: 0.1219, Val Loss: 0.2520

Validation report for BatchNorm:

	precision	recall	f1-score	support
0	0.9571	0.9902	0.9734	3378
1	0.9375	0.9474	0.9424	285
2	0.9815	0.8928	0.9350	774
3	0.5714	0.0702	0.1250	57
accuracy			0.9591	4494
macro avg	0.8619	0.7251	0.7440	4494
weighted avg	0.9552	0.9591	0.9540	4494

Test report for BatchNorm:

	precision	recall	f1-score	support
0	0.9560	0.9908	0.9731	3378
1	0.9313	0.9476	0.9393	286
2	0.9871	0.8887	0.9353	773
3	0.3333	0.0351	0.0635	57
accuracy			0.9584	4494
macro avg	0.8019	0.7156	0.7278	4494
weighted avg	0.9519	0.9584	0.9529	4494

Training model with BatchNorm_Dropout_0.5...

Epoch 1/50 - Train Loss: 1.1573, Val Loss: 0.7322
Epoch 5/50 - Train Loss: 0.3000, Val Loss: 0.2714
Epoch 10/50 - Train Loss: 0.2642, Val Loss: 0.2390
Epoch 15/50 - Train Loss: 0.2601, Val Loss: 0.2376
Epoch 20/50 - Train Loss: 0.2587, Val Loss: 0.2315
Epoch 25/50 - Train Loss: 0.2411, Val Loss: 0.2027
Epoch 30/50 - Train Loss: 0.2216, Val Loss: 0.1957
Epoch 35/50 - Train Loss: 0.2141, Val Loss: 0.1899
Epoch 40/50 - Train Loss: 0.2076, Val Loss: 0.1856
Epoch 45/50 - Train Loss: 0.2040, Val Loss: 0.1813
Epoch 50/50 - Train Loss: 0.2057, Val Loss: 0.1840
Warning: deep_L3_widths_256_128_64_32_16_reg_BatchNorm_Dropout_0.5 made no predictions for classes: [3]

Validation report for BatchNorm_Dropout_0.5:

	precision	recall	f1-score	support
0	0.9439	0.9763	0.9598	3378
1	0.7670	0.9123	0.8333	285
2	0.9970	0.8514	0.9185	774
3	0.0000	0.0000	0.0000	57
accuracy			0.9384	4494
macro avg	0.6770	0.6850	0.6779	4494
weighted avg	0.9299	0.9384	0.9325	4494

Warning: Unnamed model made no predictions for classes: [3]

Test report for BatchNorm_Dropout_0.5:

	precision	recall	f1-score	support
0	0.9403	0.9737	0.9567	3378
1	0.7507	0.9161	0.8252	286
2	0.9969	0.8344	0.9085	773
3	0.0000	0.0000	0.0000	57
accuracy			0.9337	4494
macro avg	0.6720	0.6810	0.6726	4494
weighted avg	0.9260	0.9337	0.9279	4494

Training model with WeightDecay_1e-4...

Epoch 1/50 - Train Loss: 0.5489, Val Loss: 0.3170
Epoch 5/50 - Train Loss: 0.1510, Val Loss: 0.1631
Epoch 10/50 - Train Loss: 0.1271, Val Loss: 0.1439
Epoch 15/50 - Train Loss: 0.1215, Val Loss: 0.1586
Epoch 20/50 - Train Loss: 0.1203, Val Loss: 0.1392
Epoch 25/50 - Train Loss: 0.1184, Val Loss: 0.1354
Epoch 30/50 - Train Loss: 0.1163, Val Loss: 0.1365
Epoch 35/50 - Train Loss: 0.1121, Val Loss: 0.1270
Epoch 40/50 - Train Loss: 0.1091, Val Loss: 0.1219
Epoch 45/50 - Train Loss: 0.1089, Val Loss: 0.1196
Epoch 50/50 - Train Loss: 0.1060, Val Loss: 0.1504

Validation report for WeightDecay_1e-4:

	precision	recall	f1-score	support
0	0.9597	0.9861	0.9727	3378
1	0.9373	0.9439	0.9406	285
2	0.9615	0.9031	0.9314	774
3	0.1111	0.0175	0.0303	57

accuracy		0.9568	4494
macro avg	0.7424	0.7126	0.7187
weighted avg	0.9478	0.9568	0.9516

Test report for WeightDecay_1e-4:

	precision	recall	f1-score	support
0	0.9605	0.9864	0.9733	3378
1	0.9347	0.9510	0.9428	286
2	0.9628	0.9030	0.9319	773
3	0.4444	0.0702	0.1212	57
accuracy			0.9582	4494
macro avg	0.8256	0.7276	0.7423	4494
weighted avg	0.9527	0.9582	0.9534	4494

Training model with WeightDecay_1e-4_BN_Dropout_0.5...

Epoch 1/50 - Train Loss: 1.1633, Val Loss: 0.7591

Epoch 5/50 - Train Loss: 0.3033, Val Loss: 0.2591

Epoch 10/50 - Train Loss: 0.2457, Val Loss: 0.2026

Epoch 15/50 - Train Loss: 0.2223, Val Loss: 0.1836

Epoch 20/50 - Train Loss: 0.2097, Val Loss: 0.1825

Epoch 25/50 - Train Loss: 0.2018, Val Loss: 0.1758

Epoch 30/50 - Train Loss: 0.1962, Val Loss: 0.1740

Epoch 35/50 - Train Loss: 0.2034, Val Loss: 0.1717

Epoch 40/50 - Train Loss: 0.1986, Val Loss: 0.1721

Epoch 45/50 - Train Loss: 0.1963, Val Loss: 0.1724

Epoch 50/50 - Train Loss: 0.1910, Val Loss: 0.1711

Warning: deep_L3_widths_256_128_64_32_16_reg_WeightDecay_1e-4_BN_Dropout_0.5
made no predictions for classes: [3]

Validation report for WeightDecay_1e-4_BN_Dropout_0.5:

	precision	recall	f1-score	support
0	0.9465	0.9737	0.9599	3378
1	0.7542	0.9474	0.8398	285
2	0.9970	0.8514	0.9185	774
3	0.0000	0.0000	0.0000	57
accuracy			0.9386	4494
macro avg	0.6744	0.6931	0.6795	4494
weighted avg	0.9310	0.9386	0.9330	4494

Warning: Unnamed model made no predictions for classes: [3]

```
Test report for WeightDecay_1e-4_BN_Dropout_0.5:
      precision    recall  f1-score   support

          0       0.9433    0.9710    0.9570     3378
          1       0.7378    0.9545    0.8323      286
          2       0.9985    0.8357    0.9099     773
          3       0.0000    0.0000    0.0000      57

   accuracy                           0.9344    4494
  macro avg       0.6699    0.6903    0.6748    4494
weighted avg       0.9278    0.9344    0.9288    4494
```

1.7.2 Evaluating

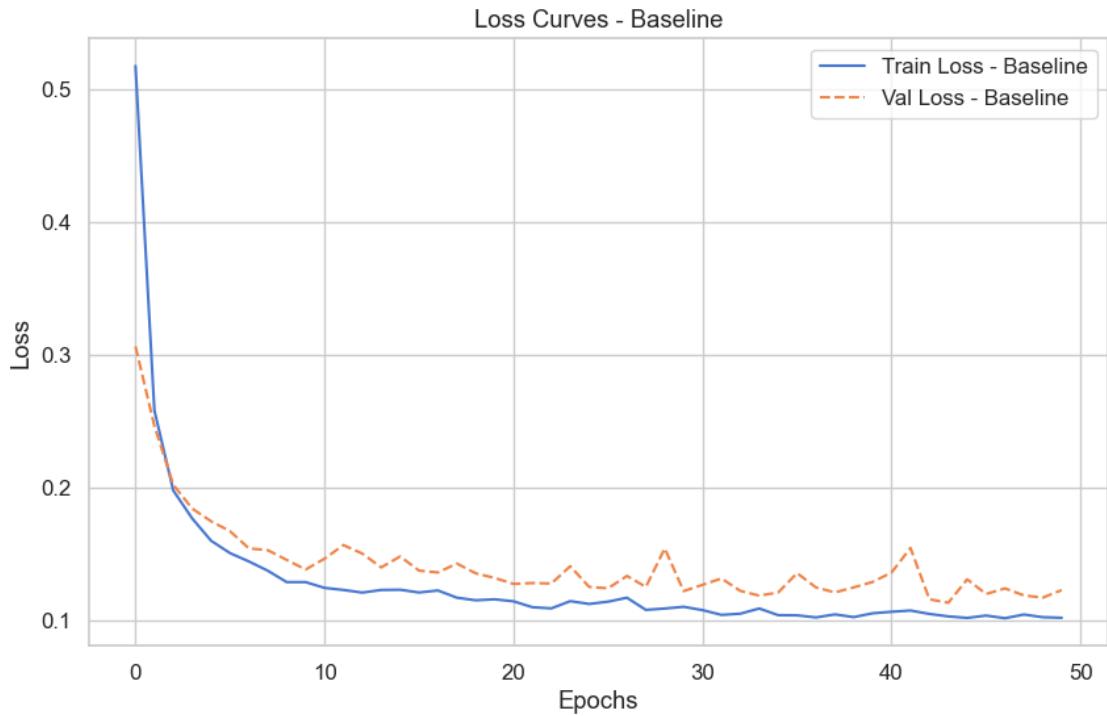
```
[135]: # --- Plot loss curves for all regularized models ---

for config_name, (train_loss, val_loss) in regularized_loss_curves.items():
    plt.figure(figsize=(10,6))
    plt.plot(train_loss, label=f'Train Loss - {config_name}')
    plt.plot(val_loss, '--', label=f'Val Loss - {config_name}')
    plt.xlabel('Epochs')
    plt.ylabel('Loss')
    plt.title(f'Loss Curves - {config_name}')
    plt.legend()

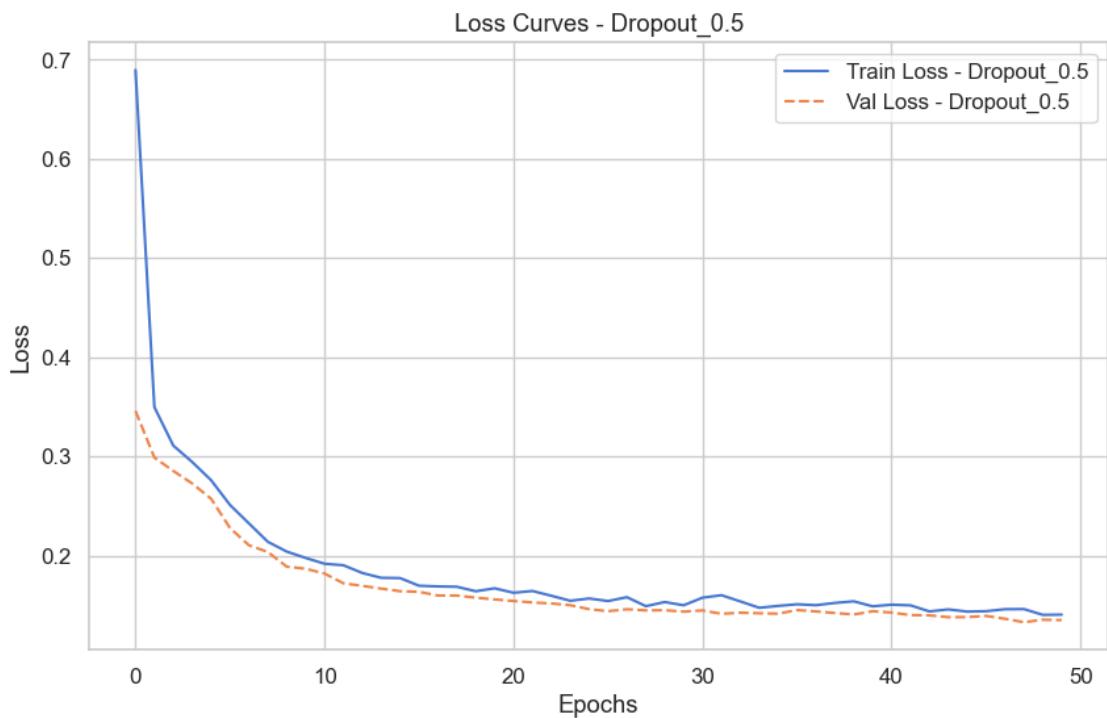
    # Save the plot to the specified path
    save_plot(plt.gcf(), f"{config_name}_loss_curve", save_dir) # Use plt.gcf() to get the current figure

plt.show()
```

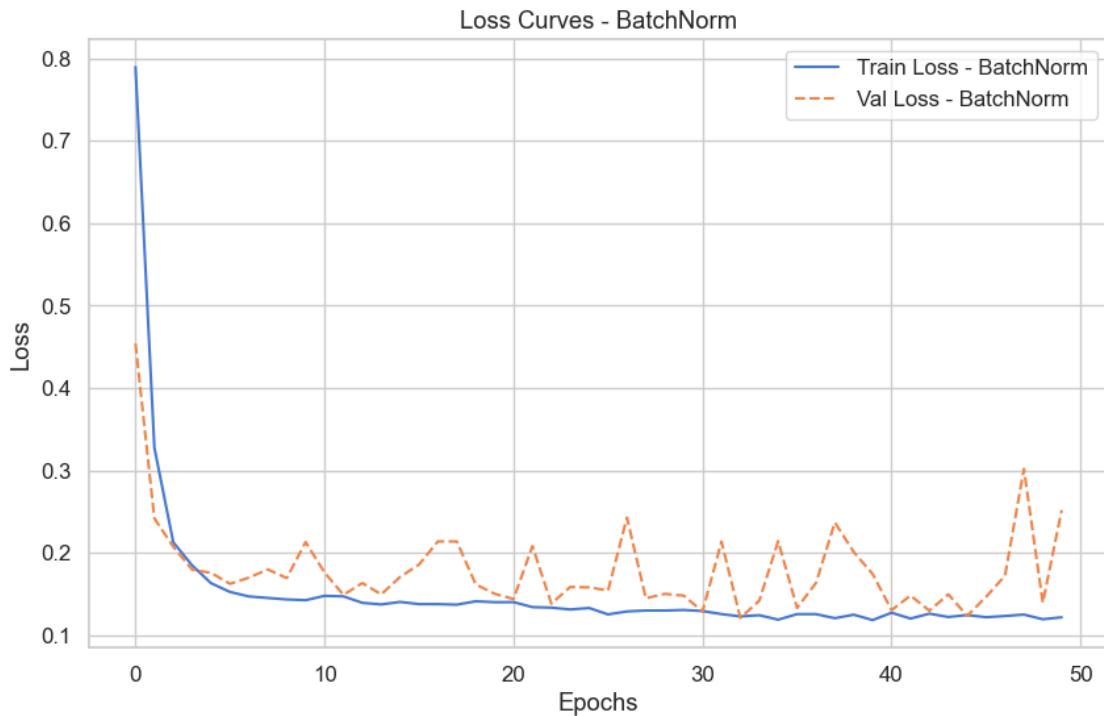
Saved plot: ../results/images/task6_plots/Baseline_loss_curve.png



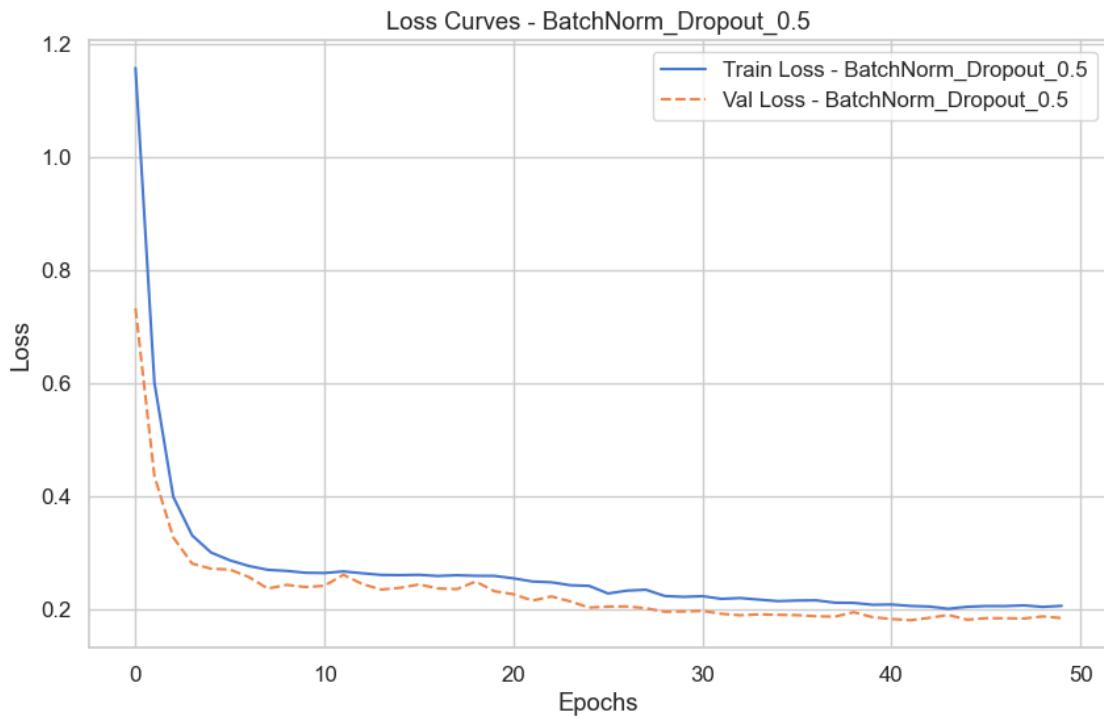
Saved plot: ./results/images/task6_plots/Dropout_0.5_loss_curve.png



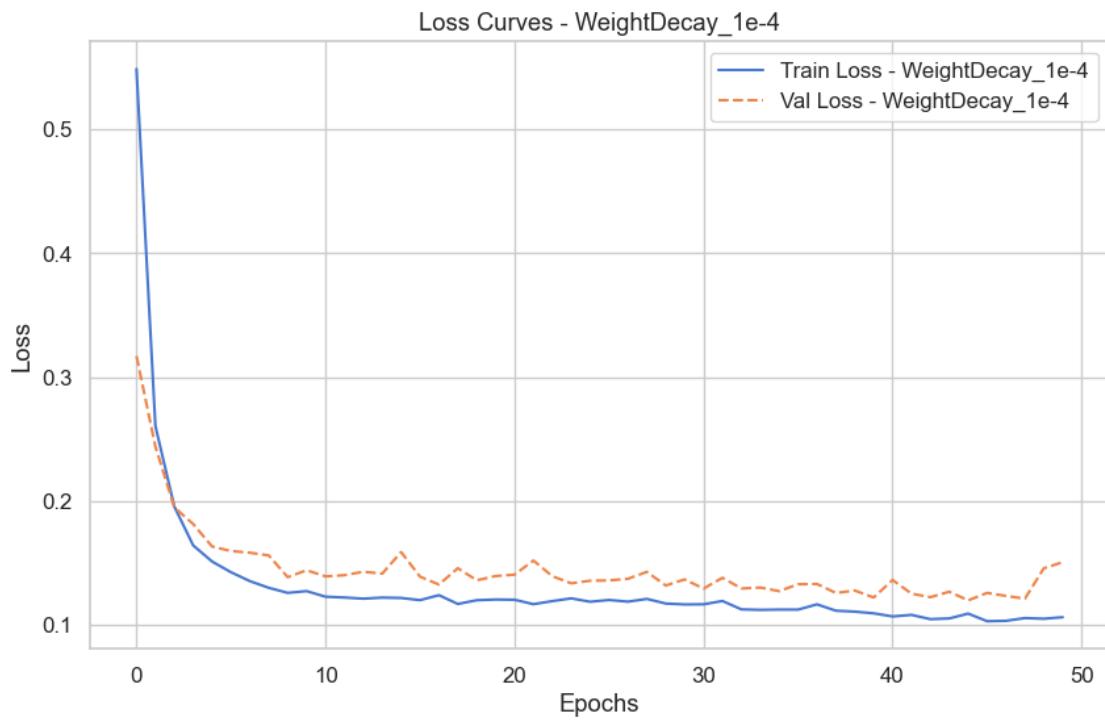
Saved plot: ../results/images/task6_plots/BatchNorm_loss_curve.png



Saved plot: ../results/images/task6_plots/BatchNorm_Dropout_0.5_loss_curve.png

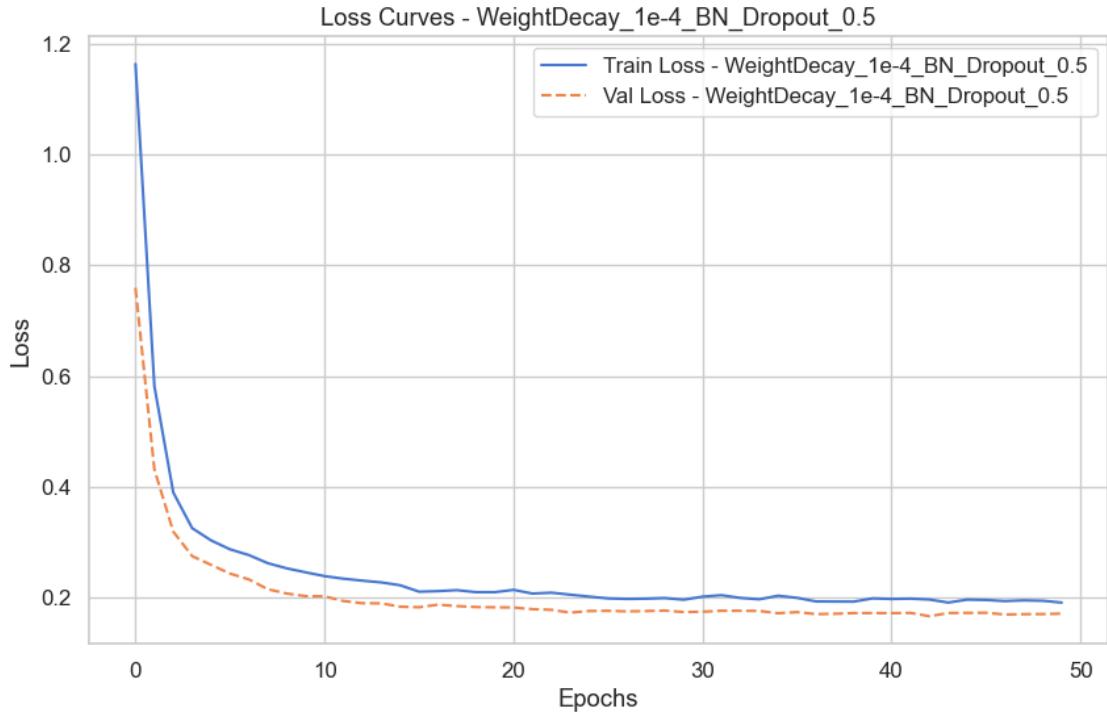


Saved plot: ../results/images/task6_plots/WeightDecay_1e-4_loss_curve.png



Saved plot:

../results/images/task6_plots/WeightDecay_1e-4_BN_Dropout_0.5_loss_curve.png



Q: Each Neurons per Layer describes how many neurons must be present in each layer. For example: 1st layer 256, 2nd layer 128 etc. What do the losses look like? Is the model overfitting? The training and validation losses both decrease smoothly and stabilize around 0.10-0.12, showing consistent convergence. The validation loss stays slightly higher than the training loss, which is expected — this indicates good generalization rather than overfitting.

If the model were overfitting, we would see the training loss continue to drop while the validation loss increased or fluctuated strongly. Here, both curves follow the same trend and plateau together.

The losses show a healthy training process — the model converges well and does not overfit, maintaining high validation accuracy (~96%).

Q: Now apply normalization techniques (dropout, batch normalization) and play with the regularization of the weights (AdamW's weight decay). What impact do the different normalization techniques have on validation and testing performance? Impact summary:

- **Baseline (AdamW)** - Best overall (Val 96%, Test 96%). Smooth convergence, no overfitting, and correct predictions for all classes.
- **Dropout (0.5)** - Validation loss a bit lower than training; minority class (3) never predicted.
- **BatchNorm** - Validation loss unstable, signs of overfitting/instability; poor minority class recall.

- **BatchNorm + Dropout (0.5)** - Too much regularization → strong underfitting; class 3 ignored.
- **Weight Decay (1e-4)** - Slightly improves generalization and keeps losses stable; close to baseline.
- **Weight Decay + BN + Dropout (0.5)** - Over-regularized; underfits, poor validation.

Best setup: *AdamW + small weight decay (1e-4)*.

Too strong: *Dropout / BatchNorm* on this tabular dataset → underfitting, unstable validation.
