Task 3g GAT model

March 26, 2024

0.1 Import Libraries

[1]:

```
!pip install torch-geometric

import os
import numpy as np
import pyarrow as pa
import pandas as pd
import pyarrow.parquet as pq
import pickle

import torch
import torch.nn as nn
import torch.nn.functional as F
from torch_geometric.nn import GATConv, global_mean_pool
from torch_geometric.data import Data, DataLoader
from sklearn.metrics import roc_curve, roc_auc_score
from scipy.spatial.distance import cdist
from tqdm import tqdm
import matplotlib.pyplot as plt
```

```
Collecting torch-geometric
  Downloading torch_geometric-2.5.0-py3-none-any.whl.metadata (64 kB)
                           64.2/64.2 kB
1.8 MB/s eta 0:00:00
Requirement already satisfied: tqdm in /opt/conda/lib/python3.10/site-
packages (from torch-geometric) (4.66.1)
Requirement already satisfied: numpy in /opt/conda/lib/python3.10/site-packages
(from torch-geometric) (1.26.4)
Requirement already satisfied: scipy in /opt/conda/lib/python3.10/site-packages
(from torch-geometric) (1.11.4)
Requirement already satisfied: fsspec in /opt/conda/lib/python3.10/site-packages
(from torch-geometric) (2024.2.0)
Requirement already satisfied: jinja2 in /opt/conda/lib/python3.10/site-packages
(from torch-geometric) (3.1.2)
Requirement already satisfied: aiohttp in /opt/conda/lib/python3.10/site-
packages (from torch-geometric) (3.9.1)
Requirement already satisfied: requests in /opt/conda/lib/python3.10/site-
```

```
packages (from torch-geometric) (2.31.0)
Requirement already satisfied: pyparsing in /opt/conda/lib/python3.10/site-
packages (from torch-geometric) (3.1.1)
Requirement already satisfied: scikit-learn in /opt/conda/lib/python3.10/site-
packages (from torch-geometric) (1.2.2)
Requirement already satisfied: psutil>=5.8.0 in /opt/conda/lib/python3.10/site-
packages (from torch-geometric) (5.9.3)
Requirement already satisfied: attrs>=17.3.0 in /opt/conda/lib/python3.10/site-
packages (from aiohttp->torch-geometric) (23.2.0)
Requirement already satisfied: multidict<7.0,>=4.5 in
/opt/conda/lib/python3.10/site-packages (from aiohttp->torch-geometric) (6.0.4)
Requirement already satisfied: yarl<2.0,>=1.0 in /opt/conda/lib/python3.10/site-
packages (from aiohttp->torch-geometric) (1.9.3)
Requirement already satisfied: frozenlist>=1.1.1 in
/opt/conda/lib/python3.10/site-packages (from aiohttp->torch-geometric) (1.4.1)
Requirement already satisfied: aiosignal>=1.1.2 in
/opt/conda/lib/python3.10/site-packages (from aiohttp->torch-geometric) (1.3.1)
Requirement already satisfied: async-timeout<5.0,>=4.0 in
/opt/conda/lib/python3.10/site-packages (from aiohttp->torch-geometric) (4.0.3)
Requirement already satisfied: MarkupSafe>=2.0 in
/opt/conda/lib/python3.10/site-packages (from jinja2->torch-geometric) (2.1.3)
Requirement already satisfied: charset-normalizer<4,>=2 in
/opt/conda/lib/python3.10/site-packages (from requests->torch-geometric) (3.3.2)
Requirement already satisfied: idna<4,>=2.5 in /opt/conda/lib/python3.10/site-
packages (from requests->torch-geometric) (3.6)
Requirement already satisfied: urllib3<3,>=1.21.1 in
/opt/conda/lib/python3.10/site-packages (from requests->torch-geometric)
(1.26.18)
Requirement already satisfied: certifi>=2017.4.17 in
/opt/conda/lib/python3.10/site-packages (from requests->torch-geometric)
(2024.2.2)
Requirement already satisfied: joblib>=1.1.1 in /opt/conda/lib/python3.10/site-
packages (from scikit-learn->torch-geometric) (1.3.2)
Requirement already satisfied: threadpoolctl>=2.0.0 in
/opt/conda/lib/python3.10/site-packages (from scikit-learn->torch-geometric)
(3.2.0)
Downloading torch_geometric-2.5.0-py3-none-any.whl (1.1 MB)
                          1.1/1.1 MB
16.5 MB/s eta 0:00:00a 0:00:01
Installing collected packages: torch-geometric
Successfully installed torch-geometric-2.5.0
```

0.2 Disable Warnings

```
[2]: import warnings
     warnings.filterwarnings("ignore")
     warnings.simplefilter("ignore")
```

0.3 Load Data

[3]:
```
def read_file(path):
  chunk_size = 25

# Create a Parquet file reader object
  parquet_file = pq.ParquetFile(path)

# Determine the total number of rows in the file
  total_rows = parquet_file.metadata.num_rows

# Loop over the file in chunks
  data = []
  for i in range(0, total_rows, chunk_size):
    # Read a chunk of rows from the file
      chunk = (parquet_file.read_row_group(i))
      dm = (chunk.to_pandas())
      data.append(dm)

# Concatenate all the DataFrames into a single DataFrame
  df = pd.concat(data, ignore_index=True)
  print(parquet_file.read_row_group(0).to_pandas())
  return df
```

[4]:
```
df1 = read_file('/kaggle/input/common-task-2-dataset/Task - 2 Data (Parquet)/
 ↪jet0_run0.test.snappy.parquet')
df2 = read_file('/kaggle/input/common-task-2-dataset/Task - 2 Data (Parquet)/
 ↪jet0_run1.test.snappy.parquet')
df3 = read_file('/kaggle/input/common-task-2-dataset/Task - 2 Data (Parquet)/
 ↪jet0_run2.test.snappy.parquet')
```

```
                                              X_jets          pt         m0  \
0  [[[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0…  112.411095  21.098248

     y
0  0.0
                                              X_jets          pt         m0  \
0  [[[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0…  147.686737  32.114449

     y
0  0.0
                                              X_jets          pt         m0  \
0  [[[0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0…  107.854118  18.723455

     y
0  0.0
```

[5]:

```
def construct_image_dataset(df):
    # Get the total number of samples
    num_samples = len(df)

    # Initialize empty arrays for X and y
    X = np.empty((num_samples, 3, 125, 125), dtype=np.float32)
    y = np.empty(num_samples, dtype=int)

    # Iterate through the DataFrame and fill X and y
    for i, row in df.iterrows():
        # Stack the three channels of X_jets and transpose them to match the␣
 ↪desired shape
        X[i] = np.transpose(np.dstack((np.stack(row['X_jets'][0]), np.
 ↪stack(row['X_jets'][1]), np.stack(row['X_jets'][2]))), (2, 0, 1))
        # Assign the label to y
        y[i] = row['y']

    # Rearrange the dimensions of X to match the TensorFlow format (samples,␣
 ↪height, width, channels)
    X = np.transpose(X, (0, 2, 3, 1))

    return X, y
```

[6]:

```
# Assuming 'df' is the pandas DataFrame
X1, y1 = construct_image_dataset(df1)
X2, y2 = construct_image_dataset(df2)
X3, y3 = construct_image_dataset(df3)
```

[7]:

```
# Save X1 array to binary file 'X1.npy'
with open('X1.npy', 'wb') as f:
    np.save(f, X1)

# Save y1 array to binary file 'y1.npy'
with open('y1.npy', 'wb') as f:
    np.save(f, y1)

# Save X2 array to binary file 'X2.npy'
with open('X2.npy', 'wb') as f:
    np.save(f, X2)

# Save y2 array to binary file 'y2.npy'
with open('y2.npy', 'wb') as f:
    np.save(f, y2)

# Save X3 array to binary file 'X3.npy'
with open('X3.npy', 'wb') as f:
    np.save(f, X3)
```

```
# Save y3 array to binary file 'y3.npy'
with open('y3.npy', 'wb') as f:
    np.save(f, y3)
```

[8]:

```
x1 = np.load('X1.npy')
x2 = np.load('X2.npy')
x3 = np.load('X3.npy')

y1 = np.load('y1.npy')
y2 = np.load('y2.npy')
y3 = np.load('y3.npy')
```

[9]:

```
# Combine x arrays along the first axis (axis=0)
x = np.concatenate((x1, x2, x3), axis=0)

# Combine y arrays along the first axis (axis=0)
y = np.concatenate((y1, y2, y3), axis=0)

# Save the combined X array to a binary file named 'X.npy'
with open('x.npy', 'wb') as f:
    np.save(f, x)

# Save the combined y array to a binary file named 'y.npy'
with open('y.npy', 'wb') as f:
    np.save(f, y)
```

[10]:

```
# Load the dataset
X = np.load("x.npy")
y = np.load("y.npy")

# Convert the numpy arrays to PyTorch tensors
X = torch.tensor(X, dtype=torch.float)
y = torch.tensor(y, dtype=torch.int)
```

[11]:

```
def linear_kernel(distance_matrix, gamma=None):
    if gamma is None:
        gamma = 1.0 / distance_matrix.shape[1]
    return gamma * np.dot(distance_matrix, gamma)

def construct_graph_using_linear_kernel(image, label):
    height, width, channels = image.shape
    nodes = []
    positions = []

    # Iterate over the 5x5 crops and extract features
    for i in range(0, height, 5):
        for j in range(0, width, 5):
            crop = image[i:i+5, j:j+5]
            feature = crop.reshape(-1)
            nodes.append(feature)
            positions.append((i, j))

    nodes = torch.stack(nodes)
    positions = np.array(positions)

    # Compute edge_index and edge_attr using Linear Kernel
    distance_matrix = cdist(positions, positions)
    linear_values = linear_kernel(distance_matrix)
    edges = np.where(linear_values > 0.8)  # Adjust threshold as needed
    edge_index = torch.tensor(np.vstack(edges), dtype=torch.long)
    edge_attr = torch.tensor(linear_values[edges], dtype=torch.float)

    # Create the PyTorch Geometric Data object
    data = Data(x=nodes, edge_index=edge_index, edge_attr=edge_attr, y=torch.
 ↪tensor([label], dtype=torch.long))
    return data
```

[12]:
```
filename = "pyg_data_list.pkl"
if os.path.exists(filename):
    print(f"{filename} exists in the current directory.")
    with open("pyg_data_list.pkl", "rb") as file:
        pyg_data_list = pickle.load(file)
else:
    print(f"{filename} does not exist in the current directory.")
    # Create PyTorch Geometric Data objects for each image
    pyg_data_list = [construct_graph_using_linear_kernel(X[i], y[i]) for i in␣
 ↪tqdm(range(X.shape[0]), desc="Creating Data Objects")]
```

```
pyg_data_list.pkl does not exist in the current directory.

Creating Data Objects: 100%|      | 5573/5573 [01:17<00:00, 71.50it/s]
```

0.4 Splitting Data into train_dataset and test_dataset

[13]:
```
# Set up the train and test datasets
train_dataset = pyg_data_list[:int(len(pyg_data_list) * 0.75)]
test_dataset = pyg_data_list[int(len(pyg_data_list) * 0.75):]

# Set up the data loader
train_loader = DataLoader(train_dataset, batch_size=32, shuffle=True)
test_loader = DataLoader(test_dataset, batch_size=32, shuffle=False)
```

0.5 Building Graph Attention Networks (GAT) Model

[14]:
```
class GATModel(torch.nn.Module):
    def __init__(self, num_node_features, hidden_channels, num_classes):
        super(GATModel, self).__init__()
        self.conv1 = GATConv(num_node_features, hidden_channels)
        self.conv2 = GATConv(hidden_channels, hidden_channels)
        self.fc = torch.nn.Linear(hidden_channels, num_classes)

    def forward(self, data):
        x, edge_index, edge_attr, batch = data.x, data.edge_index, data.
 ↪edge_attr, data.batch
        x = F.relu(self.conv1(x, edge_index, edge_attr))
        x = F.relu(self.conv2(x, edge_index, edge_attr))
        x = global_mean_pool(x, batch)
        x = F.dropout(x, p=0.5, training=self.training)
        x = self.fc(x)
        return x
```

0.6 Set up the GAT model, loss function, and optimizer

[15]:
```
num_node_features = train_dataset[0].x.shape[1]
hidden_channels = 64
num_classes = 2

device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
model = GATModel(num_node_features, hidden_channels, num_classes).to(device)
criterion = torch.nn.CrossEntropyLoss()
optimizer = torch.optim.Adam(model.parameters(), lr=1e-3)
```

0.7 Define training and evaluation functions

[16]:
```
def train():
    model.train()
    total_loss = 0
    for data in tqdm(train_loader, desc="Training"):
        data = data.to(device)
        optimizer.zero_grad() # To Clear gradients
        out = model(data) # Perform a single forward pass
        loss = criterion(out, data.y) # Compute the loss
        loss.backward() # Deriving gradients
        optimizer.step() # Updating parameters
        total_loss += loss.item()
    return total_loss / len(train_loader)

def test(loader):
    model.eval()
    correct = 0
    y_true = []
    y_probs = []

    for data in tqdm(loader, desc="Testing"):
        data = data.to(device)
        with torch.no_grad():
            out = model(data)
        probs = F.softmax(out, dim=-1)
        pred = out.argmax(dim=-1)

        y_true.extend(data.y.tolist())
        y_probs.extend(probs[:, 1].tolist())

        correct += int((pred == data.y).sum())

    false_pr, true_pr, _ = roc_curve(y_true, y_probs)
    roc_auc = roc_auc_score(y_true, y_probs)
    accuracy = correct / len(loader.dataset)

    return accuracy, false_pr, true_pr, roc_auc
```

0.8 Function to plot ROC curve

[17]:

```
def plot_roc_curve(false_pr, true_pr, roc_auc, title="ROC curve"):
    plt.figure()
    plt.plot(false_pr, true_pr, color="darkorange", lw=2, label=f"ROC curve (AUC = {roc_auc:.4f})")
    plt.plot([0, 1], [0, 1], color="blue", lw=2, linestyle="-.")
    plt.xlim([0.0, 1.0])
    plt.ylim([0.0, 1.05])
    plt.xlabel("False Positive Rate")
    plt.ylabel("True Positive Rate")
    plt.title(title)
    plt.legend(loc="lower right")
    plt.savefig("gat-roc-curve.png")
    plt.show()
```

0.9 Train and Evaluate the model

[18]:

```
num_epochs = 50
max_auc = 0

for epoch in range(num_epochs):
    loss = train()
    train_acc, _, _, train_roc_auc = test(train_loader)
    test_acc, false_pr, true_pr, test_roc_auc = test(test_loader)
    print(f"Epoch: {epoch + 1}, Loss: {loss:.4f}, Train (Accuracy): {train_acc:.
↪4f}, Train (ROC-AUC): {train_roc_auc:.4f}, Test (Accuracy): {test_acc:.4f},␣
↪Test (ROC-AUC): {test_roc_auc:.4f}")
    if test_roc_auc > max_auc:
        max_auc = test_roc_auc
        max_false_pr, max_true_pr, = false_pr, true_pr

plot_roc_curve(max_false_pr, max_true_pr, max_auc, title="ROC curve (Test set)")
```

```
Training: 100%|          | 131/131 [00:02<00:00, 54.78it/s]
Testing: 100%|          | 131/131 [00:01<00:00, 128.27it/s]
Testing: 100%|          | 44/44 [00:00<00:00, 130.57it/s]

Epoch: 1, Loss: 0.6926, Train (Accuracy): 0.5085, Train (ROC-AUC): 0.5845, Test
(Accuracy): 0.5100, Test (ROC-AUC): 0.5720

Training: 100%|          | 131/131 [00:01<00:00, 98.34it/s]
Testing: 100%|          | 131/131 [00:00<00:00, 134.60it/s]
Testing: 100%|          | 44/44 [00:00<00:00, 130.74it/s]

Epoch: 2, Loss: 0.6926, Train (Accuracy): 0.5085, Train (ROC-AUC): 0.6549, Test
(Accuracy): 0.5108, Test (ROC-AUC): 0.6336

Training: 100%|          | 131/131 [00:01<00:00, 100.39it/s]
Testing: 100%|          | 131/131 [00:01<00:00, 126.91it/s]
Testing: 100%|          | 44/44 [00:00<00:00, 103.56it/s]

Epoch: 3, Loss: 0.6902, Train (Accuracy): 0.6068, Train (ROC-AUC): 0.6720, Test
(Accuracy): 0.6011, Test (ROC-AUC): 0.6506

Training: 100%|          | 131/131 [00:01<00:00, 99.02it/s]
Testing: 100%|          | 131/131 [00:00<00:00, 132.99it/s]
Testing: 100%|          | 44/44 [00:00<00:00, 131.92it/s]

Epoch: 4, Loss: 0.6806, Train (Accuracy): 0.6420, Train (ROC-AUC): 0.6927, Test
(Accuracy): 0.6105, Test (ROC-AUC): 0.6679

Training: 100%|          | 131/131 [00:01<00:00, 102.30it/s]
Testing: 100%|          | 131/131 [00:00<00:00, 134.01it/s]
Testing: 100%|          | 44/44 [00:00<00:00, 134.43it/s]

Epoch: 5, Loss: 0.6653, Train (Accuracy): 0.6557, Train (ROC-AUC): 0.7077, Test
(Accuracy): 0.6212, Test (ROC-AUC): 0.6788

Training: 100%|          | 131/131 [00:01<00:00, 102.13it/s]
Testing: 100%|          | 131/131 [00:00<00:00, 132.43it/s]
Testing: 100%|          | 44/44 [00:00<00:00, 132.44it/s]

Epoch: 6, Loss: 0.6488, Train (Accuracy): 0.6633, Train (ROC-AUC): 0.7200, Test
(Accuracy): 0.6313, Test (ROC-AUC): 0.6891
```

```
Training: 100%|     | 131/131 [00:01<00:00, 99.27it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 131.73it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 137.00it/s]

Epoch: 7, Loss: 0.6354, Train (Accuracy): 0.6700, Train (ROC-AUC): 0.7311, Test
(Accuracy): 0.6277, Test (ROC-AUC): 0.6970

Training: 100%|     | 131/131 [00:01<00:00, 100.79it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 134.52it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 131.61it/s]

Epoch: 8, Loss: 0.6280, Train (Accuracy): 0.6791, Train (ROC-AUC): 0.7384, Test
(Accuracy): 0.6435, Test (ROC-AUC): 0.7031

Training: 100%|     | 131/131 [00:01<00:00, 101.33it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 135.23it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 137.05it/s]

Epoch: 9, Loss: 0.6210, Train (Accuracy): 0.6815, Train (ROC-AUC): 0.7455, Test
(Accuracy): 0.6428, Test (ROC-AUC): 0.7098

Training: 100%|     | 131/131 [00:01<00:00, 102.39it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 136.03it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 136.48it/s]

Epoch: 10, Loss: 0.6179, Train (Accuracy): 0.6927, Train (ROC-AUC): 0.7506, Test
(Accuracy): 0.6506, Test (ROC-AUC): 0.7149

Training: 100%|     | 131/131 [00:01<00:00, 101.88it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 132.60it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 133.15it/s]

Epoch: 11, Loss: 0.6113, Train (Accuracy): 0.6961, Train (ROC-AUC): 0.7563, Test
(Accuracy): 0.6593, Test (ROC-AUC): 0.7195

Training: 100%|     | 131/131 [00:01<00:00, 104.57it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 134.78it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 132.48it/s]

Epoch: 12, Loss: 0.6107, Train (Accuracy): 0.7021, Train (ROC-AUC): 0.7621, Test
(Accuracy): 0.6571, Test (ROC-AUC): 0.7215

Training: 100%|     | 131/131 [00:01<00:00, 104.65it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 135.15it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 134.31it/s]

Epoch: 13, Loss: 0.6048, Train (Accuracy): 0.7045, Train (ROC-AUC): 0.7667, Test
(Accuracy): 0.6600, Test (ROC-AUC): 0.7239

Training: 100%|     | 131/131 [00:01<00:00, 103.55it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 135.38it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 132.67it/s]

Epoch: 14, Loss: 0.5974, Train (Accuracy): 0.7078, Train (ROC-AUC): 0.7711, Test
(Accuracy): 0.6714, Test (ROC-AUC): 0.7275
```

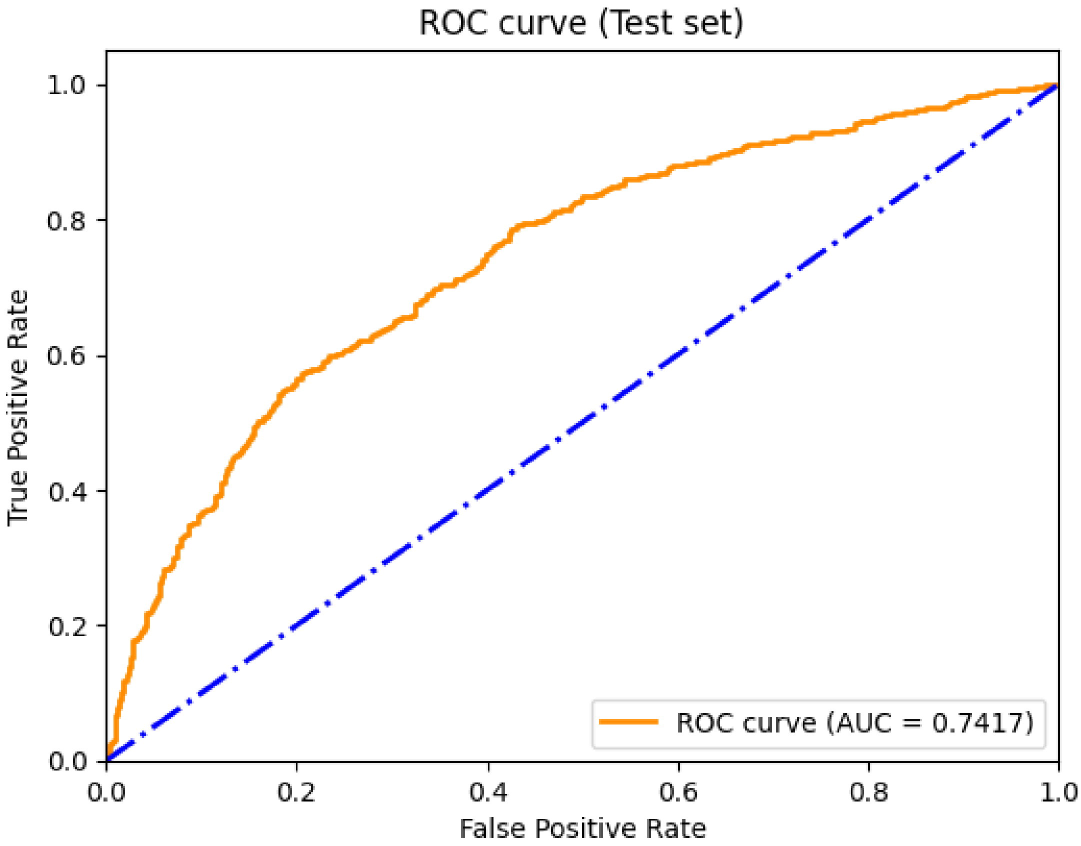
```
Training: 100%|      | 131/131 [00:01<00:00, 102.72it/s]
Testing: 100%|      | 131/131 [00:01<00:00, 123.14it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 114.67it/s]

Epoch: 15, Loss: 0.5921, Train (Accuracy): 0.7109, Train (ROC-AUC): 0.7763, Test
(Accuracy): 0.6650, Test (ROC-AUC): 0.7291

Training: 100%|      | 131/131 [00:01<00:00, 102.71it/s]
Testing: 100%|      | 131/131 [00:00<00:00, 134.84it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 134.08it/s]

Epoch: 16, Loss: 0.5902, Train (Accuracy): 0.7124, Train (ROC-AUC): 0.7809, Test
(Accuracy): 0.6650, Test (ROC-AUC): 0.7317

Training: 100%|      | 131/131 [00:01<00:00, 103.71it/s]
Testing: 100%|      | 131/131 [00:00<00:00, 135.74it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 132.62it/s]

Epoch: 17, Loss: 0.5906, Train (Accuracy): 0.7200, Train (ROC-AUC): 0.7845, Test
(Accuracy): 0.6679, Test (ROC-AUC): 0.7353

Training: 100%|      | 131/131 [00:01<00:00, 103.29it/s]
Testing: 100%|      | 131/131 [00:00<00:00, 134.32it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 126.99it/s]

Epoch: 18, Loss: 0.5823, Train (Accuracy): 0.7241, Train (ROC-AUC): 0.7863, Test
(Accuracy): 0.6707, Test (ROC-AUC): 0.7371

Training: 100%|      | 131/131 [00:01<00:00, 100.03it/s]
Testing: 100%|      | 131/131 [00:00<00:00, 134.80it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 130.00it/s]

Epoch: 19, Loss: 0.5841, Train (Accuracy): 0.7291, Train (ROC-AUC): 0.7884, Test
(Accuracy): 0.6693, Test (ROC-AUC): 0.7364

Training: 100%|      | 131/131 [00:01<00:00, 102.35it/s]
Testing: 100%|      | 131/131 [00:00<00:00, 135.47it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 133.82it/s]

Epoch: 20, Loss: 0.5773, Train (Accuracy): 0.7246, Train (ROC-AUC): 0.7937, Test
(Accuracy): 0.6758, Test (ROC-AUC): 0.7371

Training: 100%|      | 131/131 [00:01<00:00, 102.08it/s]
Testing: 100%|      | 131/131 [00:00<00:00, 134.41it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 135.33it/s]

Epoch: 21, Loss: 0.5744, Train (Accuracy): 0.7255, Train (ROC-AUC): 0.7969, Test
(Accuracy): 0.6822, Test (ROC-AUC): 0.7389

Training: 100%|      | 131/131 [00:01<00:00, 102.67it/s]
Testing: 100%|      | 131/131 [00:00<00:00, 133.82it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 132.22it/s]

Epoch: 22, Loss: 0.5695, Train (Accuracy): 0.7315, Train (ROC-AUC): 0.7969, Test
(Accuracy): 0.6750, Test (ROC-AUC): 0.7392
```

```
Training: 100%|      | 131/131 [00:01<00:00, 96.69it/s]
Testing: 100%|      | 131/131 [00:00<00:00, 132.57it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 127.09it/s]

Epoch: 23, Loss: 0.5694, Train (Accuracy): 0.7306, Train (ROC-AUC): 0.7999, Test
(Accuracy): 0.6793, Test (ROC-AUC): 0.7405

Training: 100%|      | 131/131 [00:01<00:00, 99.95it/s]
Testing: 100%|      | 131/131 [00:00<00:00, 131.89it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 138.69it/s]

Epoch: 24, Loss: 0.5691, Train (Accuracy): 0.7387, Train (ROC-AUC): 0.8035, Test
(Accuracy): 0.6858, Test (ROC-AUC): 0.7414

Training: 100%|      | 131/131 [00:01<00:00, 100.29it/s]
Testing: 100%|      | 131/131 [00:00<00:00, 134.82it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 135.02it/s]

Epoch: 25, Loss: 0.5663, Train (Accuracy): 0.7413, Train (ROC-AUC): 0.8048, Test
(Accuracy): 0.6707, Test (ROC-AUC): 0.7403

Training: 100%|      | 131/131 [00:01<00:00, 99.66it/s]
Testing: 100%|      | 131/131 [00:00<00:00, 131.30it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 126.75it/s]

Epoch: 26, Loss: 0.5631, Train (Accuracy): 0.7428, Train (ROC-AUC): 0.8088, Test
(Accuracy): 0.6815, Test (ROC-AUC): 0.7417

Training: 100%|      | 131/131 [00:01<00:00, 102.10it/s]
Testing: 100%|      | 131/131 [00:01<00:00, 123.16it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 137.69it/s]

Epoch: 27, Loss: 0.5608, Train (Accuracy): 0.7452, Train (ROC-AUC): 0.8118, Test
(Accuracy): 0.6758, Test (ROC-AUC): 0.7385

Training: 100%|      | 131/131 [00:01<00:00, 100.37it/s]
Testing: 100%|      | 131/131 [00:00<00:00, 133.08it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 135.30it/s]

Epoch: 28, Loss: 0.5567, Train (Accuracy): 0.7411, Train (ROC-AUC): 0.8150, Test
(Accuracy): 0.6872, Test (ROC-AUC): 0.7402

Training: 100%|      | 131/131 [00:01<00:00, 100.93it/s]
Testing: 100%|      | 131/131 [00:00<00:00, 132.49it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 136.16it/s]

Epoch: 29, Loss: 0.5531, Train (Accuracy): 0.7504, Train (ROC-AUC): 0.8150, Test
(Accuracy): 0.6765, Test (ROC-AUC): 0.7409

Training: 100%|      | 131/131 [00:01<00:00, 100.87it/s]
Testing: 100%|      | 131/131 [00:00<00:00, 131.13it/s]
Testing: 100%|      | 44/44 [00:00<00:00, 134.42it/s]

Epoch: 30, Loss: 0.5497, Train (Accuracy): 0.7487, Train (ROC-AUC): 0.8165, Test
(Accuracy): 0.6722, Test (ROC-AUC): 0.7407
```

```
Training: 100%|     | 131/131 [00:01<00:00, 99.46it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 132.75it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 132.55it/s]

Epoch: 31, Loss: 0.5492, Train (Accuracy): 0.7499, Train (ROC-AUC): 0.8209, Test
(Accuracy): 0.6786, Test (ROC-AUC): 0.7380

Training: 100%|     | 131/131 [00:01<00:00, 99.33it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 131.84it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 135.24it/s]

Epoch: 32, Loss: 0.5428, Train (Accuracy): 0.7533, Train (ROC-AUC): 0.8224, Test
(Accuracy): 0.6743, Test (ROC-AUC): 0.7415

Training: 100%|     | 131/131 [00:01<00:00, 103.58it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 135.33it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 129.76it/s]

Epoch: 33, Loss: 0.5399, Train (Accuracy): 0.7514, Train (ROC-AUC): 0.8221, Test
(Accuracy): 0.6765, Test (ROC-AUC): 0.7417

Training: 100%|     | 131/131 [00:01<00:00, 99.37it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 133.35it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 134.30it/s]

Epoch: 34, Loss: 0.5399, Train (Accuracy): 0.7578, Train (ROC-AUC): 0.8250, Test
(Accuracy): 0.6758, Test (ROC-AUC): 0.7410

Training: 100%|     | 131/131 [00:01<00:00, 104.49it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 136.40it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 133.47it/s]

Epoch: 35, Loss: 0.5389, Train (Accuracy): 0.7598, Train (ROC-AUC): 0.8294, Test
(Accuracy): 0.6722, Test (ROC-AUC): 0.7379

Training: 100%|     | 131/131 [00:01<00:00, 101.50it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 135.91it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 130.71it/s]

Epoch: 36, Loss: 0.5331, Train (Accuracy): 0.7550, Train (ROC-AUC): 0.8289, Test
(Accuracy): 0.6693, Test (ROC-AUC): 0.7390

Training: 100%|     | 131/131 [00:01<00:00, 100.07it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 132.92it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 136.17it/s]

Epoch: 37, Loss: 0.5330, Train (Accuracy): 0.7614, Train (ROC-AUC): 0.8321, Test
(Accuracy): 0.6779, Test (ROC-AUC): 0.7347

Training: 100%|     | 131/131 [00:01<00:00, 101.86it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 135.80it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 134.43it/s]

Epoch: 38, Loss: 0.5291, Train (Accuracy): 0.7619, Train (ROC-AUC): 0.8364, Test
(Accuracy): 0.6844, Test (ROC-AUC): 0.7365
```

```
Training: 100%|     | 131/131 [00:01<00:00, 103.00it/s]
Testing: 100%|     | 131/131 [00:01<00:00, 117.19it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 124.54it/s]

Epoch: 39, Loss: 0.5271, Train (Accuracy): 0.7583, Train (ROC-AUC): 0.8391, Test
(Accuracy): 0.6693, Test (ROC-AUC): 0.7334

Training: 100%|     | 131/131 [00:01<00:00, 102.70it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 134.78it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 133.19it/s]

Epoch: 40, Loss: 0.5237, Train (Accuracy): 0.7722, Train (ROC-AUC): 0.8396, Test
(Accuracy): 0.6750, Test (ROC-AUC): 0.7365

Training: 100%|     | 131/131 [00:01<00:00, 102.39it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 136.97it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 132.66it/s]

Epoch: 41, Loss: 0.5252, Train (Accuracy): 0.7636, Train (ROC-AUC): 0.8430, Test
(Accuracy): 0.6700, Test (ROC-AUC): 0.7328

Training: 100%|     | 131/131 [00:01<00:00, 100.81it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 135.35it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 133.47it/s]

Epoch: 42, Loss: 0.5217, Train (Accuracy): 0.7717, Train (ROC-AUC): 0.8436, Test
(Accuracy): 0.6793, Test (ROC-AUC): 0.7351

Training: 100%|     | 131/131 [00:01<00:00, 100.23it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 135.39it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 135.31it/s]

Epoch: 43, Loss: 0.5218, Train (Accuracy): 0.7698, Train (ROC-AUC): 0.8471, Test
(Accuracy): 0.6693, Test (ROC-AUC): 0.7320

Training: 100%|     | 131/131 [00:01<00:00, 101.30it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 136.28it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 138.35it/s]

Epoch: 44, Loss: 0.5151, Train (Accuracy): 0.7767, Train (ROC-AUC): 0.8465, Test
(Accuracy): 0.6765, Test (ROC-AUC): 0.7327

Training: 100%|     | 131/131 [00:01<00:00, 101.94it/s]
Testing: 100%|     | 131/131 [00:01<00:00, 127.38it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 134.14it/s]

Epoch: 45, Loss: 0.5159, Train (Accuracy): 0.7741, Train (ROC-AUC): 0.8473, Test
(Accuracy): 0.6793, Test (ROC-AUC): 0.7344

Training: 100%|     | 131/131 [00:01<00:00, 100.06it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 136.61it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 128.70it/s]

Epoch: 46, Loss: 0.5098, Train (Accuracy): 0.7803, Train (ROC-AUC): 0.8501, Test
(Accuracy): 0.6808, Test (ROC-AUC): 0.7349
```

```
Training: 100%|     | 131/131 [00:01<00:00, 100.69it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 133.26it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 136.86it/s]

Epoch: 47, Loss: 0.5104, Train (Accuracy): 0.7827, Train (ROC-AUC): 0.8529, Test
(Accuracy): 0.6743, Test (ROC-AUC): 0.7305

Training: 100%|     | 131/131 [00:01<00:00, 103.21it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 131.34it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 132.09it/s]

Epoch: 48, Loss: 0.5049, Train (Accuracy): 0.7849, Train (ROC-AUC): 0.8541, Test
(Accuracy): 0.6758, Test (ROC-AUC): 0.7293

Training: 100%|     | 131/131 [00:01<00:00, 104.35it/s]
Testing: 100%|     | 131/131 [00:01<00:00, 129.66it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 133.18it/s]

Epoch: 49, Loss: 0.5057, Train (Accuracy): 0.7861, Train (ROC-AUC): 0.8568, Test
(Accuracy): 0.6758, Test (ROC-AUC): 0.7275

Training: 100%|     | 131/131 [00:01<00:00, 104.80it/s]
Testing: 100%|     | 131/131 [00:00<00:00, 135.90it/s]
Testing: 100%|     | 44/44 [00:00<00:00, 135.99it/s]

Epoch: 50, Loss: 0.5025, Train (Accuracy): 0.7619, Train (ROC-AUC): 0.8513, Test
(Accuracy): 0.6815, Test (ROC-AUC): 0.7372
```


ROC curve (Test set)
True Positive Rate
False Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.2
0.4
0.6
0.8
1.0
ROC curve (AUC = 0.7417)