Multi_Class_Bi_GRU_Bahdanau_Attention_Glove300d_PubMedBert

April 13, 2025

Classification of Biomedical Texts with Deep Learning: LSTM, GRU, and Self-Attention

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In this section, we leverage PubMedBERT to generate contextualized embeddings and GloVe (300-dimensional) for static word representations. We further integrate a Bahdanau attention mechanism within a bidirectional GRU-based architecture to enhance the model's ability to focus on relevant textual features.

[1]:
```python
import pandas as pd
import nltk
import pickle
import random
from collections import defaultdict
from collections import Counter
import os
import time
import re

from tqdm import tqdm
import numpy as np
import torch
import wandb

import matplotlib.pyplot as plt
from sklearn.metrics import precision_score
import seaborn as sns

import torch
import torch.nn as nn
from collections import Counter
import torch.optim as optim
from google.colab import files
from google.colab import drive
from torch.optim.lr_scheduler import ReduceLROnPlateau
from torch.utils.data import Dataset, DataLoader
from torch.optim.lr_scheduler import ReduceLROnPlateau
from torch.utils.data.dataset import ConcatDataset
from sklearn.metrics import accuracy_score, f1_score
from sklearn.model_selection import train_test_split
from torch.utils.data import DataLoader, TensorDataset
from sklearn.preprocessing import LabelEncoder
from torch.nn.utils.rnn import pad_sequence

from transformers import AutoTokenizer, AutoModel
from sklearn.metrics import accuracy_score, f1_score
from torch.optim.lr_scheduler import StepLR

from sklearn.preprocessing import label_binarize
from nltk.corpus import stopwords
from sklearn.metrics import f1_score, confusion_matrix, balanced_accuracy_score,␣
 ↪precision_score, recall_score
from sklearn.metrics import classification_report, confusion_matrix,␣
 ↪ConfusionMatrixDisplay
```

[2]:
```
# To ensure reproducibility of the results
SEED = 200
random.seed(SEED)
np.random.seed(SEED)
torch.manual_seed(SEED)
torch.cuda.manual_seed(SEED)
torch.backends.cudnn.deterministic = True
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
```

[5]:
```
drive.mount('/content/drive')
```

```
Drive already mounted at /content/drive; to attempt to forcibly remount, call
drive.mount("/content/drive", force_remount=True).
```

[6]:
```
data = pd.read_csv('/content/drive/MyDrive/diseases_dataset.csv')

print(data.info())
print()

data["Label"].value_counts()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 38652 entries, 0 to 38651
Data columns (total 10 columns):
 #   Column              Non-Null Count  Dtype
---  ------              --------------  -----
 0   PMID                38652 non-null  int64
 1   Title               38652 non-null  object
 2   Abstract            38652 non-null  object
 3   Keywords            38652 non-null  object
 4   PublicationYear     38652 non-null  int64
 5   MeSH_Terms          38652 non-null  object
 6   Cleaned_Abstract    38652 non-null  object
 7   Disease             38652 non-null  object
 8   Top_Relevant_Words  38652 non-null  object
 9   Label               38652 non-null  int64
dtypes: int64(3), object(7)
memory usage: 2.9+ MB
None
```

[6]:
```
Label
6    4730
7    4658
1    4639
0    4636
4    4550
8    4503
5    4452
2    3883
3    2601
Name: count, dtype: int64
```

[ ]:
```
print(data.isna().sum())
```

```
PMID                  0
Title                 0
Abstract              0
Keywords              0
PublicationYear       0
MeSH_Terms            0
Cleaned_Abstract      0
```

```
Disease               0
Top_Relevant_Words    0
Label                 0
dtype: int64
```

[ ]:
```
data.tail()
```

[ ]:
```
           PMID                                              Title  \
38647  36360604  Analysis of the Number and Type of Vaccination...
38648  37547521  Clinicopathologic Spectrum of Lysozyme-Associa...
38649  39584999  Cystic Fibrosis Screening Efficacy and Seasona...
38650  39664903  Induction of CD4 T cell memory responses follo...
38651  32325950  Pathogenesis of Uveitis in Ebola Virus Disease...

                                                Abstract  \
38647  Vaccination is a very common topic, but it is ...
38648  INTRODUCTION: Lysozyme-associated nephropathy ...
38649  The California Genetic Disease Screening Progr...
38650  Mycobacterium bovis, the causative agent of bo...
38651  Ebola virus disease (EVD) and emerging infecti...

                                                Keywords  PublicationYear  \
38647  ['infectious diseases', 'military (soldiers)',...             2022
38648  ['chronic myelomonocytic leukemia', 'granuloma...             2023
38649  ['CF', 'DNA', 'IRT', 'cystic fibrosis', 'false...             2024
38650  ['BCG', 'CD4', 'T helper 1', 'cattle', 'immuno...             2024
38651  ['Ebola virus disease', 'animal models', 'emer...             2020

                                              MeSH_Terms  \
38647  ['Humans', '*Military Personnel', 'Poland', 'T...
38648                                                 []
38649                                                 []
38650                                                 []
38651                                                 []

                                        Cleaned_Abstract          Disease  \
38647  vaccination common topic, rarely raised discus...          Cholera
38648  introduction lysozyme associated nephropathy l...          Leprosy
38649  california genetic disease screening program g...  Cystic Fibrosis
38650  mycobacterium bovis, causative agent bovine tu...     Tuberculosis
38651  ebola virus disease evd emerging infectious di...            Ebola

                                      Top_Relevant_Words  Label
38647  ['vaccination', 'military', 'immunized', 'hepa...      1
38648  ['kidney', 'egfr', 'aki', 'min', '15', 'etiolo...      2
38649  ['cutoff', 'irt', 'seasonal', 'missed', 'cf', ...      8
38650  ['btb', 'bcg', 'bovis', 'vaccine', 'cattle', '...      0
```

```
 38651  ['evd', 'eye', 'uveitis', 'ebola', 'vision', '...      3
```

[7]:
```
X = data["Cleaned_Abstract"].values
y = data["Label"].values

# Split into training (70%), validation (15%), and test (15%) sets
X_train, X_temp, y_train, y_temp = train_test_split(X, y, test_size=0.3,␣
 ↪random_state=42)
X_val, X_test, y_val, y_test = train_test_split(X_temp, y_temp, test_size=0.5,␣
 ↪random_state=42)

print(f"Training set: {len(X_train)} samples")
print(f"Validation set: {len(X_val)} samples")
print(f"Test set: {len(X_test)} samples")

NUM_CLASSES = len(set(y))
print(NUM_CLASSES)
```

```
Training set: 27056 samples
Validation set: 5798 samples
Test set: 5798 samples
9
```

[ ]:
```
print("Training set class distribution:", Counter(y_train))
print("Validation set class distribution:", Counter(y_val))
print("Test set class distribution:", Counter(y_test))
```

```
Training set class distribution: Counter({np.int64(6): 3352, np.int64(7): 3285,
np.int64(1): 3249, np.int64(0): 3215, np.int64(4): 3213, np.int64(8): 3177,
np.int64(5): 3064, np.int64(2): 2705, np.int64(3): 1796})
Validation set class distribution: Counter({np.int64(7): 711, np.int64(0): 708,
np.int64(1): 706, np.int64(5): 680, np.int64(6): 672, np.int64(8): 672,
np.int64(4): 666, np.int64(2): 571, np.int64(3): 412})
Test set class distribution: Counter({np.int64(0): 713, np.int64(5): 708,
np.int64(6): 706, np.int64(1): 684, np.int64(4): 671, np.int64(7): 662,
np.int64(8): 654, np.int64(2): 607, np.int64(3): 393})
```

Bahdanau attention mechanism within a bidirectional GRU-based architecture

[8]:
```
# --- PubMedBERT Setup ---
pubmedbert_model_name = "microsoft/
 ↪BiomedNLP-PubMedBERT-base-uncased-abstract-fulltext"
tokenizer = AutoTokenizer.from_pretrained(pubmedbert_model_name)
pubmedbert = AutoModel.from_pretrained(pubmedbert_model_name).to(device)

for param in pubmedbert.parameters():
    param.requires_grad = True
```

```
BATCH_SIZE = 32
```

```
/usr/local/lib/python3.11/dist-packages/huggingface_hub/utils/_auth.py:94:
UserWarning:
The secret `HF_TOKEN` does not exist in your Colab secrets.
To authenticate with the Hugging Face Hub, create a token in your settings tab
(https://huggingface.co/settings/tokens), set it as secret in your Google Colab
and restart your session.
You will be able to reuse this secret in all of your notebooks.
Please note that authentication is recommended but still optional to access
public models or datasets.
  warnings.warn(
```

```
tokenizer_config.json:   0%|          | 0.00/28.0 [00:00<?, ?B/s]
```

```
config.json:   0%|          | 0.00/385 [00:00<?, ?B/s]
```

```
vocab.txt:   0%|          | 0.00/226k [00:00<?, ?B/s]
```

```
pytorch_model.bin:   0%|          | 0.00/440M [00:00<?, ?B/s]
```

[9]:

```
class BahdanauAttention(nn.Module):
    """
    Bahdanau Attention Mechanism.

    This class implements the Bahdanau attention mechanism as described in the␣
↪paper:
    "Neural Machine Translation by Jointly Learning to Align and Translate" by␣
↪Bahdanau et al.

    Args:
        hidden_dim (int): The hidden dimension of the GRU or LSTM output.

    Attributes:
        W (nn.Linear): A linear layer for the transformation of the RNN outputs.
        v (nn.Linear): A linear layer for computing attention scores.
    """
    def __init__(self, hidden_dim):
        super(BahdanauAttention, self).__init__()
        self.W = nn.Linear(hidden_dim * 2, hidden_dim)
        self.v = nn.Linear(hidden_dim, 1, bias=False)

    def forward(self, rnn_outputs):
        """
        Apply the attention mechanism on the RNN outputs.

        Args:
            rnn_outputs (Tensor): The outputs of the RNN (GRU or LSTM).
        Returns:
            Tensor: The context vector computed by the attention mechanism.
        """
        score = torch.tanh(self.W(rnn_outputs))
        attn_weights = torch.softmax(self.v(score), dim=1)
        context = torch.sum(attn_weights * rnn_outputs, dim=1)
        return context

class PubMedBERT_GRU_Attention(nn.Module):
    """
    Model combining PubMedBERT embeddings, GRU layers, and Bahdanau Attention␣
 ↪mechanism for multi-class classification.

    Args:
        bert_dim (int): The dimension of the PubMedBERT embeddings (usually 768).
        hidden_dim (int): The hidden dimension of the GRU layer.
        num_classes (int): The number of output classes for classification␣
 ↪(default is 9 for multi-class classification).
        num_layers (int): The number of layers in the GRU (default is 1).
        dropout_prob (float): Dropout probability for regularization.

    Attributes:
        gru (nn.GRU): A bidirectional GRU layer.
        attention (BahdanauAttention): The Bahdanau attention mechanism.
        fc (nn.Linear): The fully connected layer to produce the output␣
 ↪predictions.
        dropout (nn.Dropout): Dropout layer for regularization.
    """
    def __init__(self, bert_dim, hidden_dim, num_classes=9, num_layers=1,␣
 ↪dropout_prob=0.6):
        super(PubMedBERT_GRU_Attention, self).__init__()

        self.gru = nn.GRU(
            input_size=bert_dim,
            hidden_size=hidden_dim,
            num_layers=num_layers,
            batch_first=True,
            bidirectional=True
        )

        self.attention = BahdanauAttention(hidden_dim)
        self.fc = nn.Linear(hidden_dim * 2, num_classes)
        self.dropout = nn.Dropout(dropout_prob)

    def forward(self, input_ids, attention_mask):
        """
        Forward pass of the model.

        Args:
            input_ids (Tensor): The tokenized input sequence IDs.
            attention_mask (Tensor): The attention mask to differentiate padding␣
↪from real tokens.

        Returns:
            Tensor: The output logits for classification.
        """
        with torch.no_grad():
            bert_outputs = pubmedbert(input_ids=input_ids,␣
↪attention_mask=attention_mask)
        bert_embeds = bert_outputs.last_hidden_state
        gru_out, _ = self.gru(bert_embeds)
        context = self.attention(gru_out)
        x = self.dropout(context)
        output = self.fc(x)  # Logits for multi-class classification
        return output
```

[10]:
```
def count_parameters(model):
    """
    Count the number of trainable parameters in the model.
    Args:
        model: The model whose parameters are to be counted.
    Returns:
        Total number of trainable parameters.
    """
    return sum(p.numel() for p in model.parameters() if p.requires_grad)

def train_model(model, dataloader, optimizer, criterion, device):
    """
    Train the model for one epoch, calculating loss and accuracy.
    Args:
        model: The model to train.
        dataloader: DataLoader for the training dataset.
        optimizer: Optimizer for model parameters.
        criterion: Loss function.
        device: CPU/GPU device.
    Returns:
        Average loss and accuracy for the epoch.
    """
    model.train()
    total_loss = 0
    total_correct = 0
    total_samples = 0
```

```python
    for batch in dataloader:
        input_ids = batch['input_ids'].to(device)
        attention_mask = batch['attention_mask'].to(device)
        labels = batch['labels'].to(device)

        optimizer.zero_grad()
        logits = model(input_ids, attention_mask)

        loss = criterion(logits, labels)
        loss.backward()
        optimizer.step()

        total_loss += loss.item()

        preds = torch.argmax(logits, dim=1).cpu().detach().numpy()
        total_correct += np.sum(preds == labels.cpu().numpy())
        total_samples += labels.size(0)

    avg_loss = total_loss / len(dataloader)
    avg_accuracy = total_correct / total_samples
    return avg_loss, avg_accuracy

def evaluate_model(model, dataloader, criterion, device):
    """
    Validate the model for one epoch, including precision, F1, balanced␣
 ↪accuracy, and recall.
    Args:
        model: Model instance.
        dataloader: DataLoader for validation data.
        criterion: Loss function (CrossEntropyLoss).
        device: CPU/GPU.
    Returns:
        Average validation loss, accuracy, F1-score.
    """
    model.eval()
    all_preds = []
    all_labels = []
    val_loss = 0.0

    with torch.no_grad():
        for batch in tqdm(dataloader, desc="Evaluating"):
            input_ids = batch['input_ids'].to(device)
            attention_mask = batch['attention_mask'].to(device)
            labels = batch['labels'].to(device)

            logits = model(input_ids, attention_mask)
            loss = criterion(logits, labels)
            val_loss += loss.item()

            preds = torch.argmax(logits, dim=1).cpu().numpy()
            labels_cpu = labels.cpu().numpy()

            all_preds.extend(preds)
            all_labels.extend(labels_cpu)

    val_loss /= len(dataloader)
    all_preds = np.array(all_preds)
    all_labels = np.array(all_labels)

    acc = accuracy_score(all_labels, all_preds)
    f1 = f1_score(all_labels, all_preds, average="weighted")

    return acc, f1, val_loss

def test_model(model, test_loader, criterion, device):
    """
    Evaluate the model on the test dataset, calculating loss, accuracy,␣
 ↪F1-score, precision, recall, and balanced accuracy.
    Args:
        model: The model to evaluate.
        test_loader: DataLoader for the test dataset.
        criterion: Loss function (CrossEntropyLoss).
        device: CPU/GPU device.
    Returns:
        Average test loss, accuracy, F1-score, balanced accuracy, recall, and␣
 ↪precision.
    """
    model.eval()
    total_loss = 0
    total_accuracy = 0
    all_labels = []
    all_preds = []

    with torch.no_grad():
        for batch in test_loader:
            input_ids = batch['input_ids'].to(device)
            attention_mask = batch['attention_mask'].to(device)
            target_tensor = batch['labels'].to(device)

            output = model(input_ids, attention_mask)
            loss = criterion(output, target_tensor)
            total_loss += loss.item()
            batch_accuracy = accuracy_score(target_tensor.cpu(), torch.
↪argmax(output, dim=1).cpu())
            total_accuracy += batch_accuracy * len(target_tensor)

            preds = torch.argmax(output, dim=1).cpu().numpy()
            labels = target_tensor.cpu().numpy()

            all_preds.extend(preds)
            all_labels.extend(labels)

    avg_loss = total_loss / len(test_loader)
    avg_accuracy = total_accuracy / len(test_loader.dataset)
    all_preds = np.array(all_preds)
    all_labels = np.array(all_labels)

    f1 = f1_score(all_labels, all_preds, average="weighted", zero_division=0)
    balanced_acc = balanced_accuracy_score(all_labels, all_preds)
    precision = precision_score(all_labels, all_preds, average="weighted",␣
↪zero_division=0)
    recall = recall_score(all_labels, all_preds, average="weighted",␣
↪zero_division=0)

    return avg_loss, avg_accuracy, f1, balanced_acc, recall, precision
```

[11]:
```
BERT_DIM = 768
HIDDEN_DIM = 256
DROPOUT = 0.6

model = PubMedBERT_GRU_Attention(BERT_DIM, HIDDEN_DIM, dropout_prob=DROPOUT).
↪to(device)
print()
print(f"{count_parameters(model)} model parameters")
print()
print(model)
```

```

1712137 model parameters

PubMedBERT_GRU_Attention(
  (gru): GRU(768, 256, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=512, out_features=256, bias=True)
    (v): Linear(in_features=256, out_features=1, bias=False)
  )
  (fc): Linear(in_features=512, out_features=9, bias=True)
  (dropout): Dropout(p=0.6, inplace=False)
)
```

#1. Use of PubMedBERT as contextual embeddings

PubMedBERT is a model pre-trained on a corpus of biomedical texts, and generates contextual embeddings.

[12]:
```
class PubMedBERTBinaryDataset(Dataset):
    """
    Dataset class for multi-class classification using PubMedBERT embeddings.

    Args:
        texts (list of str): A list of raw text sequences.
        labels (list of int): A list of integer labels (0-8) corresponding to␣
↪each text.
        tokenizer (transformers tokenizer): A tokenizer to preprocess the text␣
↪data.
        max_length (int): Maximum length for padding/truncation. Default is 400.

    Attributes:
        texts (list of str): The raw text data.
        encodings (dict): Tokenized text data with input IDs and attention masks.
        labels (Tensor): Tensor of integer labels for the classification task.
    """

    def __init__(self, texts, labels, tokenizer, max_length=400):
        self.texts = texts
        self.encodings = tokenizer(texts, padding='max_length', truncation=True,␣
↪max_length=max_length, return_tensors='pt')
        self.labels = torch.tensor(labels, dtype=torch.long)

    def __getitem__(self, idx):
        """
        Retrieve a single sample from the dataset.

        Args:
            idx (int): Index of the sample to retrieve.

        Returns:
            dict: Contains input IDs, attention masks, and the corresponding␣
↪label and raw text.
        """
        item = {key: val[idx] for key, val in self.encodings.items()}
        item['labels'] = self.labels[idx]
        item['text'] = self.texts[idx]
        return item
    def __len__(self):
        """
        Returns the total number of samples in the dataset.

        Returns:
            int: Number of samples in the dataset.
        """
        return len(self.labels)
```

[13]:
```
# --- Load Data ---
train_dataset = PubMedBERTBinaryDataset(X_train.tolist(), y_train, tokenizer)
val_dataset = PubMedBERTBinaryDataset(X_val.tolist(), y_val, tokenizer)
test_dataset = PubMedBERTBinaryDataset(X_test.tolist(), y_test, tokenizer)

train_loader = DataLoader(train_dataset, batch_size=BATCH_SIZE, shuffle=True)
val_loader = DataLoader(val_dataset, batch_size=BATCH_SIZE, shuffle=False)
test_loader = DataLoader(test_dataset, batch_size=BATCH_SIZE, shuffle=False)

# Combine the training and validation datasets (for test)
combined_dataset = ConcatDataset([train_dataset, val_dataset])
combined_loader = DataLoader(combined_dataset, batch_size=BATCH_SIZE,␣
 ↪shuffle=True)
```

0.1 1.1 Optimisation phase

1.1.1 Optimizer selection

[ ]:
```
num_epochs = 5
learning_rate = 1e-4
weight_decay = 1e-3
criterion = torch.nn.CrossEntropyLoss()

optimizers = {
    'Adam': optim.Adam,
    'AdamW': optim.AdamW,
    'RMSprop': optim.RMSprop,
}

all_train_losses = {}
all_val_losses = {}
all_train_accs = {}
all_val_accs = {}

for optimizer_name, optimizer_class in optimizers.items():
    print(f"\n Training with optimizer: {optimizer_name}")

    model = PubMedBERT_GRU_Attention(BERT_DIM, HIDDEN_DIM, dropout_prob=DROPOUT).
↪to(device)
    print(model)

    optimizer = optimizer_class(model.parameters(), lr=learning_rate,␣
↪weight_decay=weight_decay)
    scheduler = ReduceLROnPlateau(optimizer, mode='min', factor=0.5, patience=2,␣
↪verbose=True)

    wandb.init(project='Multi_Class_Pubmedbert_Attention_OptimizerSearch',␣
↪name=f"{optimizer_name}_run", config={
        'learning_rate': learning_rate,
        'num_epochs': num_epochs,
        'optimizer': optimizer_name,
        'model': 'PubMedBERT_Bi_GRU_Bahdanau_Attention',
        'hidden_dim': HIDDEN_DIM,
        'dropout_prob': DROPOUT
    })

    num_params = sum(p.numel() for p in model.parameters() if p.requires_grad)
    print(f"Total trainable parameters: {num_params}")

    train_losses, val_losses = [], []
    train_accs, val_accs = [], []
    best_val_loss = float('inf')

    for epoch in range(num_epochs):
        start_time = time.time()

        train_loss, train_acc = train_model(model, train_loader, optimizer,␣
↪criterion, device)
        train_losses.append(train_loss)
        train_accs.append(train_acc)

        val_acc, f1, val_loss = evaluate_model(model, val_loader, criterion,␣
↪device)
        val_accs.append(val_acc)
        val_losses.append(val_loss)

        end_time = time.time()
        duration = end_time - start_time

        print(
            f"Opt: {optimizer_name} | Epoch {epoch+1}/{num_epochs} - "
            f"TL: {train_loss:.4f}, VL: {val_loss:.4f}, "
            f"TA: {train_acc:.2%}, VA: {val_acc:.2%}, F1: {f1:.2%}, "
            f"Time: {duration/60:.2f} min"
        )

        wandb.log({
            'train_loss': train_loss,
            'val_loss': val_loss,
            'train_acc': train_acc,
            'val_acc': val_acc,
            'val_f1': f1,
        })

        scheduler.step(val_loss)

    all_train_losses[optimizer_name] = train_losses
    all_val_losses[optimizer_name] = val_losses
    all_train_accs[optimizer_name] = train_accs
    all_val_accs[optimizer_name] = val_accs

    wandb.finish()
```

Adam optimizer is selected.

1.1.2 Depth value selection

```
[ ]: depth_values = [1, 2, 3]
num_epochs = 5
learning_rate = 1e-4
weight_decay = 1e-3
criterion = torch.nn.CrossEntropyLoss()

all_train_losses = {}
all_val_losses = {}
all_train_accs = {}
all_val_accs = {}

for depth in depth_values:
    print(f"\n Training with GRU depth: {depth}")

    model = PubMedBERT_GRU_Attention(
        bert_dim=BERT_DIM,
        hidden_dim=HIDDEN_DIM,
        num_classes=9,
        num_layers=depth,
        dropout_prob=DROPOUT
    ).to(device)
    optimizer = optim.Adam(model.parameters(), lr=learning_rate,␣
↪weight_decay=weight_decay)
    scheduler = ReduceLROnPlateau(optimizer, mode='min', factor=0.5, patience=2,␣
↪verbose=True)

    wandb.init(
        project='Multi_Class_Pubmedbert_Attention_DepthSearch',
        name=f"Depth_{depth}_run",
        config={
            'learning_rate': learning_rate,
            'num_epochs': num_epochs,
            'optimizer': 'Adam',
            'gru_depth': depth,
            'model': 'PubMedBERT_Bi_GRU_Bahdanau_Attention',
            'hidden_dim': HIDDEN_DIM,
            'dropout_prob': DROPOUT
        }
    )

    num_params = sum(p.numel() for p in model.parameters() if p.requires_grad)
    print(f"Total trainable parameters (depth={depth}): {num_params}")

    train_losses, val_losses = [], []
    train_accs, val_accs = [], []
    best_val_loss = float('inf')

    for epoch in range(num_epochs):
        start_time = time.time()

        train_loss, train_acc = train_model(model, train_loader, optimizer,␣
↪criterion, device)
        val_acc, f1, val_loss = evaluate_model(model, val_loader, criterion,␣
↪device)

        train_losses.append(train_loss)
        train_accs.append(train_acc)
        val_losses.append(val_loss)
        val_accs.append(val_acc)

        end_time = time.time()
        duration = end_time - start_time

        print(
            f"Depth: {depth} | Epoch {epoch+1}/{num_epochs} - "
            f"TL: {train_loss:.4f}, VL: {val_loss:.4f}, "
            f"TA: {train_acc:.2%}, VA: {val_acc:.2%}, F1: {f1:.2%}, "
            f"Time: {duration/60:.2f} min"
        )

        wandb.log({
            'train_loss': train_loss,
            'val_loss': val_loss,
            'train_acc': train_acc,
            'val_acc': val_acc,
            'val_f1': f1,
        })

        scheduler.step(val_loss)

    all_train_losses[f'depth_{depth}'] = train_losses
    all_val_losses[f'depth_{depth}'] = val_losses
    all_train_accs[f'depth_{depth}'] = train_accs
    all_val_accs[f'depth_{depth}'] = val_accs

    wandb.finish()
```

```
 Training with GRU depth: 1
```

```
wandb: Using wandb-core as the SDK backend.  Please refer to
https://wandb.me/wandb-core for more information.
```

```
<IPython.core.display.Javascript object>
```

```
wandb: Logging into wandb.ai. (Learn how to deploy a W&B server
locally: https://wandb.me/wandb-server)
wandb: You can find your API key in your browser here:
https://wandb.ai/authorize
wandb: Paste an API key from your profile and hit enter:
```

```
 ··········
```

```
wandb: WARNING If you're specifying your api key in code,
ensure this code is not shared publicly.
wandb: WARNING Consider setting the WANDB_API_KEY
environment variable, or running `wandb login` from the command line.
wandb: No netrc file found, creating one.
wandb: Appending key for api.wandb.ai to your netrc file:
/root/.netrc
wandb: Currently logged in as: wilfried-mvomoeto
(wilfried-mvomoeto-university-of-li-ge) to
https://api.wandb.ai. Use `wandb login --relogin` to force
relogin
```

```
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```

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Total trainable parameters (depth=1): 1712137

Training: 100%|| 846/846 [10:32<00:00,  1.34it/s]
Evaluating: 100%|| 182/182 [02:09<00:00,  1.41it/s]

Depth: 1 | Epoch 1/5 - TL: 0.7334, VL: 0.2954, TA: 77.97%, VA: 91.26%, F1:
91.14%, Time: 12.69 min

Training: 100%|| 846/846 [10:32<00:00,  1.34it/s]
Evaluating: 100%|| 182/182 [02:09<00:00,  1.41it/s]

Depth: 1 | Epoch 2/5 - TL: 0.2679, VL: 0.2730, TA: 91.96%, VA: 91.31%, F1:
91.30%, Time: 12.70 min

Training: 100%|| 846/846 [10:32<00:00,  1.34it/s]
Evaluating: 100%|| 182/182 [02:09<00:00,  1.41it/s]

Depth: 1 | Epoch 3/5 - TL: 0.2448, VL: 0.2652, TA: 92.36%, VA: 91.43%, F1:
91.37%, Time: 12.69 min

Training: 100%|| 846/846 [10:32<00:00,  1.34it/s]
Evaluating: 100%|| 182/182 [02:09<00:00,  1.41it/s]

Depth: 1 | Epoch 4/5 - TL: 0.2336, VL: 0.2640, TA: 92.73%, VA: 91.79%, F1:
91.75%, Time: 12.69 min

Training: 100%|| 846/846 [10:31<00:00,  1.34it/s]
Evaluating: 100%|| 182/182 [02:08<00:00,  1.41it/s]

Depth: 1 | Epoch 5/5 - TL: 0.2249, VL: 0.2615, TA: 93.00%, VA: 91.86%, F1:
91.81%, Time: 12.68 min


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 Training with GRU depth: 2

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Total trainable parameters (depth=2): 2894857
```

```
Training: 100%|| 846/846 [11:07<00:00,  1.27it/s]
Evaluating: 100%|| 182/182 [02:12<00:00,  1.38it/s]

Depth: 2 | Epoch 1/5 - TL: 0.6391, VL: 0.3060, TA: 80.28%, VA: 90.50%, F1:
90.47%, Time: 13.33 min

Training: 100%|| 846/846 [11:07<00:00,  1.27it/s]
Evaluating: 100%|| 182/182 [02:11<00:00,  1.38it/s]

Depth: 2 | Epoch 2/5 - TL: 0.2703, VL: 0.2834, TA: 91.84%, VA: 90.81%, F1:
90.87%, Time: 13.32 min

Training: 100%|| 846/846 [11:07<00:00,  1.27it/s]
Evaluating: 100%|| 182/182 [02:11<00:00,  1.38it/s]

Depth: 2 | Epoch 3/5 - TL: 0.2452, VL: 0.2563, TA: 92.37%, VA: 91.76%, F1:
91.74%, Time: 13.32 min

Training: 100%|| 846/846 [11:07<00:00,  1.27it/s]
Evaluating: 100%|| 182/182 [02:11<00:00,  1.39it/s]

Depth: 2 | Epoch 4/5 - TL: 0.2342, VL: 0.2704, TA: 92.65%, VA: 91.51%, F1:
91.43%, Time: 13.31 min

Training: 100%|| 846/846 [11:07<00:00,  1.27it/s]
Evaluating: 100%|| 182/182 [02:12<00:00,  1.38it/s]

Depth: 2 | Epoch 5/5 - TL: 0.2249, VL: 0.2533, TA: 92.95%, VA: 92.03%, F1:
92.02%, Time: 13.32 min


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 Training with GRU depth: 3

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Total trainable parameters (depth=3): 4077577

Training: 100%|| 846/846 [11:40<00:00,  1.21it/s]
Evaluating: 100%|| 182/182 [02:14<00:00,  1.35it/s]
```

```
Depth: 3 | Epoch 1/5 - TL: 0.6080, VL: 0.3145, TA: 81.07%, VA: 90.62%, F1:
90.58%, Time: 13.92 min

Training: 100%|| 846/846 [11:40<00:00,  1.21it/s]
Evaluating: 100%|| 182/182 [02:14<00:00,  1.35it/s]

Depth: 3 | Epoch 2/5 - TL: 0.2809, VL: 0.3050, TA: 91.36%, VA: 90.89%, F1:
90.79%, Time: 13.91 min

Training: 100%|| 846/846 [11:40<00:00,  1.21it/s]
Evaluating: 100%|| 182/182 [02:14<00:00,  1.36it/s]

Depth: 3 | Epoch 3/5 - TL: 0.2576, VL: 0.2698, TA: 92.01%, VA: 91.20%, F1:
91.22%, Time: 13.90 min

Training: 100%|| 846/846 [11:39<00:00,  1.21it/s]
Evaluating: 100%|| 182/182 [02:14<00:00,  1.35it/s]

Depth: 3 | Epoch 4/5 - TL: 0.2467, VL: 0.2730, TA: 92.29%, VA: 91.39%, F1:
91.36%, Time: 13.91 min

Training: 100%|| 846/846 [11:40<00:00,  1.21it/s]
Evaluating: 100%|| 182/182 [02:13<00:00,  1.36it/s]

Depth: 3 | Epoch 5/5 - TL: 0.2355, VL: 0.2644, TA: 92.50%, VA: 91.70%, F1:
91.62%, Time: 13.90 min


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```

Depth value is set to 2.

1.3 Leanring rate value selection

```
[ ]: learning_rates = [9e-5, 7e-5, 5e-5]
     num_epochs = 5
     criterion = torch.nn.CrossEntropyLoss()

     all_train_losses = {}
     all_val_losses = {}
     all_train_accs = {}
     all_val_accs = {}

     for lr in learning_rates:
         print(f"\n Training with learning rate: {lr}")
```

```
    model = PubMedBERT_GRU_Attention(
        bert_dim=BERT_DIM,
        hidden_dim=HIDDEN_DIM,
        num_classes=9,
        num_layers=2,
        dropout_prob=DROPOUT
    ).to(device)

    optimizer = optim.Adam(model.parameters(), lr=lr, weight_decay=1e-3)
    scheduler = ReduceLROnPlateau(optimizer, mode='min', factor=0.5, patience=2,␣
↪verbose=True)

    wandb.init(
        project='Multi_Class_Pubmedbert_Attention_LRTuning',
        name=f"LR_{lr}_run",
        config={
            'learning_rate': lr,
            'num_epochs': num_epochs,
            'optimizer': 'Adam',
            'gru_depth': depth,
            'model': 'PubMedBERT_Bi_GRU_Bahdanau_Attention',
            'hidden_dim': HIDDEN_DIM,
            'dropout_prob': DROPOUT
        }
    )

    num_params = sum(p.numel() for p in model.parameters() if p.requires_grad)
    print(f"Total trainable parameters (lr={lr}): {num_params}")

    train_losses, val_losses = [], []
    train_accs, val_accs = [], []
    best_val_loss = float('inf')

    for epoch in range(num_epochs):
        start_time = time.time()

        train_loss, train_acc = train_model(model, train_loader, optimizer,␣
↪criterion, device)
        val_acc, f1, val_loss = evaluate_model(model, val_loader, criterion,␣
↪device)

        train_losses.append(train_loss)
        train_accs.append(train_acc)
        val_losses.append(val_loss)
        val_accs.append(val_acc)

        end_time = time.time()
        duration = end_time - start_time

        print(
            f"LR: {lr} | Epoch {epoch+1}/{num_epochs} - "
            f"TL: {train_loss:.4f}, VL: {val_loss:.4f}, "
            f"TA: {train_acc:.2%}, VA: {val_acc:.2%}, F1: {f1:.2%}, "
            f"Time: {duration/60:.2f} min"
        )

        wandb.log({
            'train_loss': train_loss,
            'val_loss': val_loss,
            'train_acc': train_acc,
            'val_acc': val_acc,
            'val_f1': f1,
        })

        scheduler.step(val_loss)

    all_train_losses[f'lr_{lr}'] = train_losses
    all_val_losses[f'lr_{lr}'] = val_losses
    all_train_accs[f'lr_{lr}'] = train_accs
    all_val_accs[f'lr_{lr}'] = val_accs

    wandb.finish()
```

```
 Training with learning rate: 9e-05

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Total trainable parameters (lr=9e-05): 2894857

Training: 100%|| 846/846 [10:39<00:00,  1.32it/s]
Evaluating: 100%|| 182/182 [02:05<00:00,  1.44it/s]

LR: 9e-05 | Epoch 1/5 - TL: 0.6746, VL: 0.2990, TA: 79.27%, VA: 90.74%, F1:
90.72%, Time: 12.76 min

Training: 100%|| 846/846 [10:38<00:00,  1.32it/s]
Evaluating: 100%|| 182/182 [02:05<00:00,  1.45it/s]

LR: 9e-05 | Epoch 2/5 - TL: 0.2705, VL: 0.2730, TA: 91.64%, VA: 91.24%, F1:
91.19%, Time: 12.75 min
```

```
Training: 100%|| 846/846 [10:38<00:00,  1.32it/s]
Evaluating: 100%|| 182/182 [02:05<00:00,  1.45it/s]

LR: 9e-05 | Epoch 3/5 - TL: 0.2500, VL: 0.2676, TA: 92.31%, VA: 91.70%, F1:
91.70%, Time: 12.74 min

Training: 100%|| 846/846 [10:38<00:00,  1.32it/s]
Evaluating: 100%|| 182/182 [02:05<00:00,  1.45it/s]

LR: 9e-05 | Epoch 4/5 - TL: 0.2352, VL: 0.2651, TA: 92.78%, VA: 91.86%, F1:
91.88%, Time: 12.74 min

Training: 100%|| 846/846 [10:38<00:00,  1.32it/s]
Evaluating: 100%|| 182/182 [02:05<00:00,  1.44it/s]

LR: 9e-05 | Epoch 5/5 - TL: 0.2273, VL: 0.2564, TA: 92.93%, VA: 92.14%, F1:
92.09%, Time: 12.75 min


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 Training with learning rate: 7e-05

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Total trainable parameters (lr=7e-05): 2894857

Training: 100%|| 846/846 [10:39<00:00,  1.32it/s]
Evaluating: 100%|| 182/182 [02:06<00:00,  1.44it/s]

LR: 7e-05 | Epoch 1/5 - TL: 0.7341, VL: 0.3170, TA: 77.93%, VA: 90.12%, F1:
90.15%, Time: 12.76 min

Training: 100%|| 846/846 [10:38<00:00,  1.32it/s]
Evaluating: 100%|| 182/182 [02:05<00:00,  1.44it/s]

LR: 7e-05 | Epoch 2/5 - TL: 0.2799, VL: 0.2788, TA: 91.41%, VA: 91.36%, F1:
91.33%, Time: 12.74 min

Training: 100%|| 846/846 [10:38<00:00,  1.32it/s]
Evaluating: 100%|| 182/182 [02:05<00:00,  1.44it/s]
```

```
LR: 7e-05 | Epoch 3/5 - TL: 0.2532, VL: 0.2708, TA: 92.19%, VA: 91.84%, F1:
91.77%, Time: 12.75 min

Training: 100%|| 846/846 [10:39<00:00,  1.32it/s]
Evaluating: 100%|| 182/182 [02:05<00:00,  1.45it/s]

LR: 7e-05 | Epoch 4/5 - TL: 0.2407, VL: 0.2615, TA: 92.51%, VA: 91.86%, F1:
91.79%, Time: 12.75 min

Training: 100%|| 846/846 [10:38<00:00,  1.32it/s]
Evaluating: 100%|| 182/182 [02:05<00:00,  1.45it/s]

LR: 7e-05 | Epoch 5/5 - TL: 0.2293, VL: 0.2712, TA: 92.86%, VA: 91.12%, F1:
91.14%, Time: 12.75 min


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 Training with learning rate: 5e-05

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Total trainable parameters (lr=5e-05): 2894857

Training: 100%|| 846/846 [10:38<00:00,  1.32it/s]
Evaluating: 100%|| 182/182 [02:05<00:00,  1.45it/s]

LR: 5e-05 | Epoch 1/5 - TL: 0.9081, VL: 0.3390, TA: 72.69%, VA: 89.57%, F1:
89.51%, Time: 12.74 min

Training: 100%|| 846/846 [10:38<00:00,  1.33it/s]
Evaluating: 100%|| 182/182 [02:05<00:00,  1.45it/s]

LR: 5e-05 | Epoch 2/5 - TL: 0.2931, VL: 0.2884, TA: 91.33%, VA: 91.12%, F1:
91.05%, Time: 12.74 min

Training: 100%|| 846/846 [10:38<00:00,  1.33it/s]
Evaluating: 100%|| 182/182 [02:05<00:00,  1.45it/s]

LR: 5e-05 | Epoch 3/5 - TL: 0.2598, VL: 0.2758, TA: 91.98%, VA: 91.45%, F1:
91.41%, Time: 12.74 min
```

```
Training: 100%|| 846/846 [10:38<00:00,  1.32it/s]
Evaluating: 100%|| 182/182 [02:05<00:00,  1.45it/s]

LR: 5e-05 | Epoch 4/5 - TL: 0.2445, VL: 0.2718, TA: 92.30%, VA: 91.43%, F1:
91.43%, Time: 12.74 min

Training: 100%|| 846/846 [10:38<00:00,  1.32it/s]
Evaluating: 100%|| 182/182 [02:05<00:00,  1.45it/s]

LR: 5e-05 | Epoch 5/5 - TL: 0.2317, VL: 0.2643, TA: 92.74%, VA: 91.57%, F1:
91.53%, Time: 12.74 min


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```

Learning rate value is set to $ 9 ·10^{−5}$.

#2. Use of Glove (300d) as word embeddings

GloVe (Global Vectors for Word Representation) is a type of word embedding developed by the Stanford NLP Group.

[14]:
```python
def tokenize(text):
    """
    Tokenizes the input text by converting it to lowercase and splitting it into␣
 ↪words.

    Args:
        text: A string containing the text to be tokenized.

    Returns:
        A list of tokens (words) from the text.
    """
    return re.findall(r'\b\w+\b', text.lower())
```

[15]:
```python
all_tokens = [token for text in X_train for token in tokenize(text)]
vocab = Counter(all_tokens)
filtered_vocab = {word: freq for word, freq in vocab.items() if freq >= 2}
VOCAB_SIZE =  40000
```

```
sorted_filtered_vocab = dict(sorted(filtered_vocab.items(), key=lambda item:␣
↪item[1], reverse=True)[:VOCAB_SIZE])

word_to_index = {word: idx for idx, (word, _) in enumerate(sorted_filtered_vocab.
↪items(), 1)}
word_to_index["<PAD>"] = 0
word_to_index["<UNK>"] = len(word_to_index)

index_to_word = {idx: word for word, idx in word_to_index.items()}
```

[16]:
```
def text_to_sequence(text):
    """
    Converts the tokenized text into a sequence of indices based on a␣
↪word-to-index mapping.

    Args:
        text: A string containing the text to be converted.

    Returns:
        A list of integers representing the sequence of token indices.
    """
    return [word_to_index.get(token, word_to_index["<UNK>"]) for token in␣
↪tokenize(text)]

def pad_to_tensor(sequences, max_len=None):
    """
    Pads sequences to the specified maximum length, or truncates them if they␣
↪exceed it.

    Args:
        sequences: A list of sequences (each sequence is a list of integers).
        max_len: The maximum length to which sequences should be padded. If␣
↪None, no padding is applied.

    Returns:
        A tensor containing the padded (or truncated) sequences.
    """
    padded_sequences = [torch.tensor(seq, dtype=torch.long) for seq in sequences]
    if max_len:
        padded_sequences = [seq[:max_len] for seq in padded_sequences]
        padded_sequences = [
            torch.cat([seq, torch.zeros(max_len - len(seq), dtype=torch.long)],␣
↪0) if len(seq) < max_len else seq
            for seq in padded_sequences
        ]
    return torch.stack(padded_sequences)

class TextDataset(Dataset):
    """
    Custom Dataset for handling text data and labels.

    Args:
        X_data: Input features (e.g., tokenized text).
        y_data: Labels corresponding to the text data.
        raw_text_data: (Optional) The raw text data for reference (default is␣
↪None).
    """
    def __init__(self, X_data, y_data, raw_text_data=None):
        self.X = torch.tensor(X_data, dtype=torch.long)
        self.y = torch.tensor(y_data, dtype=torch.long)
        self.raw_text_data = raw_text_data

    def __len__(self):
        return len(self.X)

    def __getitem__(self, idx):
        input_tensor = self.X[idx]
        target_tensor = self.y[idx]
        raw_text = self.raw_text_data[idx] if self.raw_text_data is not None␣
↪else None
        return input_tensor, target_tensor, raw_text

def load_glove_embeddings(glove_path, word_to_index, embedding_dim):
    """Loads GloVe embeddings and returns an embedding matrix."""
    embedding_matrix = np.zeros((len(word_to_index), embedding_dim),␣
↪dtype='float32')
    with open(glove_path, 'r', encoding="utf-8") as f:
        for line in f:
            values = line.strip().split()
            word = values[0]
            if word in word_to_index:
                vector = np.asarray(values[1:], dtype='float32')
                embedding_matrix[word_to_index[word]] = vector

    return torch.tensor(embedding_matrix, dtype=torch.float)
```

[17]:
```
X_train_seq = [text_to_sequence(text) for text in X_train]
X_val_seq = [text_to_sequence(text) for text in X_val]
X_test_seq = [text_to_sequence(text) for text in X_test]

print(X_train_seq[0])
max_length = 400
```

```
X_train_tensor = pad_to_tensor(X_train_seq, max_len=max_length)
X_val_tensor = pad_to_tensor(X_val_seq, max_len=max_length)
X_test_tensor = pad_to_tensor(X_test_seq, max_len=max_length)

print(f"Train Tensor Shape: {X_train_tensor.shape}, Type: {X_train_tensor.
 ↪dtype}")
print(f"Validation Tensor Shape: {X_val_tensor.shape}, Type: {X_val_tensor.
 ↪dtype}")
print(f"Test Tensor Shape: {X_test_tensor.shape}, Type: {X_test_tensor.dtype}")

y_train_tensor = torch.tensor(y_train)
y_val_tensor = torch.tensor(y_val)
y_test_tensor = torch.tensor(y_test)
```

```
[79, 347, 3, 40, 127, 119, 11, 445, 2521, 351, 89, 42, 342, 763, 7415, 333,
5299, 6666, 133, 448, 52, 18, 1464, 79, 4, 499, 295, 233, 31, 6666, 1243, 38,
18, 699, 389, 2717, 119, 11, 445, 161, 4, 2639, 611, 83, 1490, 387, 694, 112,
6666, 79, 412, 1440, 913, 557, 3331, 40001, 622, 728, 128, 4687, 909, 2871, 458,
64, 607, 4412, 219, 4, 190, 19, 7153, 8005, 190, 287, 375, 876, 74, 1354, 458,
93, 4, 229, 9, 654, 132, 6666, 233, 31, 1243, 917, 2298, 213, 38, 4283, 18, 775,
43, 114, 136, 445, 9, 337, 6666, 40, 429, 80, 11, 301, 79]
Train Tensor Shape: torch.Size([27056, 400]), Type: torch.int64
Validation Tensor Shape: torch.Size([5798, 400]), Type: torch.int64
Test Tensor Shape: torch.Size([5798, 400]), Type: torch.int64
```

[18]:
```
class GloVe_GRU_BahdanauAttention(nn.Module):
    """
    Model using GloVe embeddings, GRU layers, and Bahdanau Attention for␣
 ↪classification.

    Args:
        embedding_matrix (Tensor): Pretrained GloVe embedding matrix.
        hidden_dim (int): Hidden size for the GRU.
        num_classes (int): Output classes.
        num_layers (int): GRU depth.
        dropout_prob (float): Dropout rate.
    """
    def __init__(self, embedding_matrix, hidden_dim, num_classes=NUM_CLASSES,␣
 ↪num_layers=1, dropout_prob=0.6):
        super(GloVe_GRU_BahdanauAttention, self).__init__()

        vocab_size, embedding_dim = embedding_matrix.shape
        self.embedding = nn.Embedding.from_pretrained(embedding_matrix,␣
 ↪freeze=False)

        self.gru = nn.GRU(
            input_size=embedding_dim,
            hidden_size=hidden_dim,
            num_layers=num_layers,
            batch_first=True,
            bidirectional=True
        )

        self.attention = BahdanauAttention(hidden_dim)
        self.fc = nn.Linear(hidden_dim * 2, num_classes)
        self.dropout = nn.Dropout(dropout_prob)

    def forward(self, x):
        """
        Args:
            x (Tensor): Tensor of token indices (batch_size, seq_len)

        Returns:
            Tensor: Output logits for classification.
        """
        embedded = self.embedding(x)
        gru_out, _ = self.gru(embedded)
        context = self.attention(gru_out)
        x = self.dropout(context)
        output = self.fc(x)
        return output
```

[19]:
```
def calculate_accuracy(y_pred, y_true):
    """
    Compute classification accuracy for multi-class predictions.

    Args:
        y_pred (Tensor): Raw output logits from the model of shape (batch_size,␣
 ↪num_classes).
        y_true (Tensor): Ground truth labels of shape (batch_size,).

    Returns:
        float: Accuracy score over the batch.
    """
    preds = torch.argmax(y_pred, dim=1)
    correct = (preds == y_true).sum().item()
    total = y_true.size(0)
    return correct / total

def train_epoch_glove(model, train_loader, optimizer, criterion, device):
    """
    Train the model for one epoch on the training data using GloVe embeddings.
    Args:
        model (nn.Module): The model to be trained.
        train_loader (DataLoader): DataLoader for the training data.
        optimizer (torch.optim.Optimizer): Optimizer for training.
        criterion (nn.Module): Loss function.
        device (torch.device): Device to run the training on (CPU or CUDA).

    Returns:
        Tuple[float, float]: Average loss and accuracy over the epoch.
    """
    model.train()
    total_loss, total_accuracy = 0, 0

    for batch in train_loader:
        if len(batch) == 3:
            input_tensor, target_tensor, _ = batch  # Ignore raw_text
        input_tensor, target_tensor = input_tensor.to(device), target_tensor.
↪to(device)

        optimizer.zero_grad()
        output = model(input_tensor)

        loss = criterion(output, target_tensor)
        loss.backward()

        torch.nn.utils.clip_grad_norm_(model.parameters(), max_norm=1.0)
        optimizer.step()

        acc = calculate_accuracy(output, target_tensor)
        total_loss += loss.item()
        total_accuracy += acc * input_tensor.size(0)

    avg_loss = total_loss / len(train_loader)
    avg_accuracy = total_accuracy / len(train_loader.dataset)

    return avg_loss, avg_accuracy


def validate_epoch_glove(model, val_loader, criterion, device):
    """
    Validate the model on the validation set and compute weighted F1 and␣
↪accuracy.

    Args:
        model (nn.Module): The trained model.
        val_loader (DataLoader): DataLoader for the validation data.
        criterion (nn.Module): Loss function.
        device (torch.device): Device to run validation on.

    Returns:
        Tuple[float, float, float]: Average loss, F1 score, and accuracy.
    """
    model.eval()
    total_loss, total_accuracy = 0, 0

    all_preds = []
    all_labels = []

    with torch.no_grad():
        for batch in val_loader:
            if len(batch) == 3:
                input_tensor, target_tensor, _ = batch  # Ignore raw_text
            input_tensor, target_tensor = input_tensor.to(device), target_tensor.
 ↪to(device)

            output = model(input_tensor)  # logits

            loss = criterion(output, target_tensor)
            acc = calculate_accuracy(output, target_tensor)

            total_loss += loss.item()
            total_accuracy += acc * input_tensor.size(0)

            preds = torch.argmax(output, dim=1).cpu().numpy()
            labels = target_tensor.cpu().numpy()

            all_preds.extend(preds)
            all_labels.extend(labels)

    avg_loss = total_loss / len(val_loader)
    avg_accuracy = total_accuracy / len(val_loader.dataset)
    f1 = f1_score(all_labels, all_preds, average='weighted', zero_division=0)

    return  avg_accuracy, f1, avg_loss

def test_epoch_glove(model, val_loader, criterion, device):
    """
    Validate the model and compute a complete set of metrics for multi-class␣
 ↪classification.

    Args:
        model (nn.Module): The trained model.
        val_loader (DataLoader): DataLoader for the validation data.
        criterion (nn.Module): Loss function.
        device (torch.device): Device to run validation on.

    Returns:
        Tuple[float, float, float, float, float, float]:
            Average loss, accuracy, F1 score (weighted),
            balanced accuracy, recall (weighted), precision (weighted).
    """
    model.eval()
    total_loss, total_accuracy = 0, 0

    all_preds = []
    all_labels = []

    with torch.no_grad():
        for batch in val_loader:
            if len(batch) == 3:
                input_tensor, target_tensor, _ = batch  # Ignore raw_text
            else:
                input_tensor, target_tensor = batch

            input_tensor = input_tensor.to(device)
            target_tensor = target_tensor.to(device).long()

            output = model(input_tensor)  # logits

            loss = criterion(output, target_tensor)
            acc = calculate_accuracy(output, target_tensor)

            total_loss += loss.item()
            total_accuracy += acc * input_tensor.size(0)

            preds = torch.argmax(output, dim=1).cpu().numpy()
            labels = target_tensor.cpu().numpy()

            all_preds.extend(preds)
            all_labels.extend(labels)

    avg_loss = total_loss / len(val_loader)
    avg_accuracy = total_accuracy / len(val_loader.dataset)
    f1 = f1_score(all_labels, all_preds, average='weighted', zero_division=0)
    balanced_acc = balanced_accuracy_score(all_labels, all_preds)
    precision = precision_score(all_labels, all_preds, average='weighted',␣
↪zero_division=0)
    recall = recall_score(all_labels, all_preds, average='weighted',␣
↪zero_division=0)

    return avg_loss, avg_accuracy, f1, balanced_acc, recall, precision
```

[20]:
```
EMBEDDING_DIM = 300
embedding_matrix = load_glove_embeddings('/content/drive/MyDrive/glove/glove.6B.
 ↪300d.txt', word_to_index, EMBEDDING_DIM)

train_dataset = TextDataset(X_train_tensor, y_train, raw_text_data=X_train)
val_dataset = TextDataset(X_val_tensor, y_val, raw_text_data=X_val)
test_dataset = TextDataset(X_test_tensor, y_test, raw_text_data=X_test)

train_loader = DataLoader(train_dataset, batch_size=BATCH_SIZE, shuffle=True)
val_loader = DataLoader(val_dataset, batch_size=BATCH_SIZE, shuffle=False)
test_loader = DataLoader(test_dataset, batch_size=BATCH_SIZE, shuffle=False)
```

```
<ipython-input-16-811d6649565c>:44: UserWarning: To copy construct from a
tensor, it is recommended to use sourceTensor.clone().detach() or
sourceTensor.clone().detach().requires_grad_(True), rather than
torch.tensor(sourceTensor).
  self.X = torch.tensor(X_data, dtype=torch.long)
```

0.2 2.1 Optimisation phase

2.1.1 Optimizer selection

[ ]:
```
num_epochs = 7
learning_rate = 7e-4
loss_function = torch.nn.CrossEntropyLoss()

optimizers = {
    'RMSprop': optim.RMSprop,
    'Adam': optim.Adam,
    'AdamW': optim.AdamW,
}

for optimizer_name, optimizer_class in optimizers.items():
    print(f"\n Training with optimizer: {optimizer_name}")

    model = GloVe_GRU_BahdanauAttention(embedding_matrix=embedding_matrix,␣
 ↪hidden_dim=350, num_layers=1, dropout_prob=0.8).to(device)
    optimizer = optimizer_class(model.parameters(), lr=learning_rate)
    wandb.
 ↪init(project='Multi_Class_Optimizer_Comparison_gru_attention_glove300d',␣
 ↪name=f"{optimizer_name}_run", config={
        'learning_rate': learning_rate,
        'num_epochs': num_epochs,
        'optimizer': optimizer_name,
        'model': 'GRU_Model',
        'embedding_dim': 300,
        'hidden_dim': 350,
        'dropout_prob': 0.5
    })

    print(model)
    num_params = count_parameters(model)
    print(f"Total trainable parameters: {num_params}")

    train_losses, val_losses = [], []
    train_accs, val_accs = [], []
    val_f1s = []

    with tqdm(total=num_epochs, desc=f"Optimizer: {optimizer_name}",␣
↪unit="epoch") as pbar:
        for epoch in range(num_epochs):
            start_time = time.time()

            train_loss, train_acc = train_epoch_glove(model, train_loader,␣
↪optimizer, loss_function, device)
            train_losses.append(train_loss)
            train_accs.append(train_acc)

            val_acc, val_f1, val_loss = validate_epoch_glove(model, val_loader,␣
↪loss_function, device)
            val_losses.append(val_loss)
            val_accs.append(val_acc)
            val_f1s.append(val_f1)

            end_time = time.time()
            epoch_duration = end_time - start_time

            pbar.set_description(f"Optimizer: {optimizer_name} | Epoch {epoch+1}/
↪{num_epochs} - Train Loss: {train_loss:.4f}, Val Loss: {val_loss:.4f}, Train␣
↪ACC: {train_acc:.2%}, Val ACC: {val_acc:.2%}, Time: {epoch_duration / 60:.2f}␣
↪min")
            pbar.update(1)

            wandb.log({
                'train_loss': train_loss,
                'val_loss': val_loss,
                'train_acc': train_acc,
                'val_acc': val_acc,
                'val_f1': val_f1,
            })

    wandb.finish()
```

```
 Training with optimizer: RMSprop

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GloVe_GRU_BahdanauAttention(
  (embedding): Embedding(40002, 300)
  (gru): GRU(300, 350, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=700, out_features=350, bias=True)
    (v): Linear(in_features=350, out_features=1, bias=False)
  )
  (fc): Linear(in_features=700, out_features=9, bias=True)
  (dropout): Dropout(p=0.8, inplace=False)
)
Total trainable parameters: 13621809

Optimizer: RMSprop | Epoch 7/7 - Train Loss: 0.0788, Val Loss: 0.3216, Train
ACC: 97.70%, Val ACC: 92.05%, Time: 0.99 min: 100%|| 7/7 [07:00<00:00,
60.08s/epoch]

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 Training with optimizer: Adam

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GloVe_GRU_BahdanauAttention(
  (embedding): Embedding(40002, 300)
  (gru): GRU(300, 350, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=700, out_features=350, bias=True)
    (v): Linear(in_features=350, out_features=1, bias=False)
  )
  (fc): Linear(in_features=700, out_features=9, bias=True)
  (dropout): Dropout(p=0.8, inplace=False)
)
Total trainable parameters: 13621809

Optimizer: Adam | Epoch 7/7 - Train Loss: 0.0613, Val Loss: 0.3698, Train ACC:
98.12%, Val ACC: 91.01%, Time: 1.01 min: 100%|| 7/7 [07:03<00:00,
60.48s/epoch]

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 Training with optimizer: AdamW

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GloVe_GRU_BahdanauAttention(
  (embedding): Embedding(40002, 300)
  (gru): GRU(300, 350, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=700, out_features=350, bias=True)
    (v): Linear(in_features=350, out_features=1, bias=False)
  )
  (fc): Linear(in_features=700, out_features=9, bias=True)
  (dropout): Dropout(p=0.8, inplace=False)
)
Total trainable parameters: 13621809

Optimizer: AdamW | Epoch 7/7 - Train Loss: 0.0603, Val Loss: 0.4043, Train ACC:
98.21%, Val ACC: 91.51%, Time: 1.07 min: 100%|| 7/7 [07:18<00:00,
62.64s/epoch]

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```

```
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```

RMSprop optimizer is selected as optimizer.

2.1.2 Learning rate value selection

```
[ ]: learning_rates = [9e-5, 7e-5, 5e-5]
     optimizer_class = optim.RMSprop

     for lr in learning_rates:
         optimizer_name = "RMSprop"
         print(f"\n Training with optimizer: {optimizer_name} | Learning rate: {lr}")

         model = GloVe_GRU_BahdanauAttention(
             embedding_matrix=embedding_matrix,
             hidden_dim=300,
             num_classes=NUM_CLASSES,
             num_layers=1,
             dropout_prob=0.9
         ).to(device)

         optimizer = optimizer_class(model.parameters(), lr=lr, weight_decay = 1e-5)

         wandb.init(
             project='Multi_Class_lr_Tuning_gru_attention_glove300d',
             name=f"{optimizer_name}_lr{lr}",
             config={
                 'learning_rate': lr,
                 'num_epochs': num_epochs,
                 'optimizer': optimizer_name,
                 'model': 'GRU_Model',
                 'embedding_dim': 300,
                 'hidden_dim': 350,
                 'dropout_prob': 0.8
             }
         )

         print(model)
         num_params = count_parameters(model)
         print(f"Total trainable parameters: {num_params}")

         train_losses, val_losses = [], []
         train_accs, val_accs = [], []
         val_f1s = []

         with tqdm(total=num_epochs, desc=f"Optimizer: {optimizer_name} | LR: {lr}",␣
      ↪unit="epoch") as pbar:
             for epoch in range(num_epochs):
                 start_time = time.time()

                 train_loss, train_acc = train_epoch_glove(model, train_loader,␣
     ↪optimizer, loss_function, device)
                 train_losses.append(train_loss)
                 train_accs.append(train_acc)

                 val_acc, val_f1, val_loss = validate_epoch_glove(model, val_loader,␣
     ↪loss_function, device)
                 val_losses.append(val_loss)
                 val_accs.append(val_acc)
                 val_f1s.append(val_f1)

                 end_time = time.time()
                 epoch_duration = end_time - start_time

                 pbar.set_description(
                     f"Optimizer: {optimizer_name} | LR: {lr} | Epoch {epoch+1}/
     ↪{num_epochs} - "
                     f"Train Loss: {train_loss:.4f}, Val Loss: {val_loss:.4f}, "
                     f"Train ACC: {train_acc:.2%}, Val ACC: {val_acc:.2%}, "
                     f"F1: {val_f1:.2f}, Time: {epoch_duration / 60:.2f} min"
                 )
                 pbar.update(1)

                 wandb.log({
                     'train_loss': train_loss,
                     'val_loss': val_loss,
                     'train_acc': train_acc,
                     'val_acc': val_acc,
                     'val_f1': val_f1,
                 })

         wandb.finish()
```

```
 Training with optimizer: RMSprop | Learning rate: 9e-05

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```

```
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GloVe_GRU_BahdanauAttention(
  (embedding): Embedding(40002, 300)
  (gru): GRU(300, 300, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=600, out_features=300, bias=True)
    (v): Linear(in_features=300, out_features=1, bias=False)
  )
  (fc): Linear(in_features=600, out_features=9, bias=True)
  (dropout): Dropout(p=0.9, inplace=False)
)
Total trainable parameters: 13270209

Optimizer: RMSprop | LR: 9e-05 | Epoch 7/7 - Train Loss: 0.2407, Val Loss:
0.2638, Train ACC: 92.85%, Val ACC: 91.95%, F1: 0.92, Time: 0.81 min:
100%|| 7/7 [05:42<00:00, 48.96s/epoch]

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 Training with optimizer: RMSprop | Learning rate: 7e-05

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GloVe_GRU_BahdanauAttention(
  (embedding): Embedding(40002, 300)
  (gru): GRU(300, 300, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=600, out_features=300, bias=True)
    (v): Linear(in_features=300, out_features=1, bias=False)
  )
  (fc): Linear(in_features=600, out_features=9, bias=True)
  (dropout): Dropout(p=0.9, inplace=False)
)
Total trainable parameters: 13270209

Optimizer: RMSprop | LR: 7e-05 | Epoch 7/7 - Train Loss: 0.2456, Val Loss:
0.2706, Train ACC: 92.79%, Val ACC: 91.74%, F1: 0.92, Time: 0.81 min:
```

```
100%|| 7/7 [05:41<00:00, 48.74s/epoch]

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 Training with optimizer: RMSprop | Learning rate: 5e-05

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GloVe_GRU_BahdanauAttention(
  (embedding): Embedding(40002, 300)
  (gru): GRU(300, 300, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=600, out_features=300, bias=True)
    (v): Linear(in_features=300, out_features=1, bias=False)
  )
  (fc): Linear(in_features=600, out_features=9, bias=True)
  (dropout): Dropout(p=0.9, inplace=False)
)
Total trainable parameters: 13270209

Optimizer: RMSprop | LR: 5e-05 | Epoch 7/7 - Train Loss: 0.2579, Val Loss:
0.2693, Train ACC: 92.25%, Val ACC: 91.70%, F1: 0.92, Time: 0.81 min:
100%|| 7/7 [05:40<00:00, 48.58s/epoch]

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```

Learning rate value is set to $9 \cdot 10{-}5$.

2.1.3 Depth value selection

[ ]:
```
learning_rate = 9e-5
depth_values = [1, 2, 3]

for depth in depth_values:
    optimizer_name = "RMSprop"
    print(f"\n Training with optimizer: {optimizer_name} | Depth: {depth}")

    model = GloVe_GRU_BahdanauAttention(
        embedding_matrix=embedding_matrix,
        hidden_dim=300,
        num_classes=NUM_CLASSES,
        num_layers=depth,
        dropout_prob=0.9
    ).to(device)

    optimizer = optimizer_class(model.parameters(), lr=learning_rate)

    wandb.init(
        project='Multi_Class_Depth_Tuning_gru_attention_glove300d',
        name=f"{optimizer_name}_depth{depth}",
        config={
            'learning_rate': learning_rate,
            'num_epochs': num_epochs,
            'optimizer': optimizer_name,
            'model': 'GRU_Model',
            'embedding_dim': 300,
            'hidden_dim': 300,
            'dropout_prob': 0.9,
            'num_layers': depth
        }
    )

    print(model)
    num_params = count_parameters(model)
    print(f"Total trainable parameters: {num_params}")

    train_losses, val_losses = [], []
    train_accs, val_accs = [], []
    val_f1s = []

    with tqdm(total=num_epochs, desc=f"Optimizer: {optimizer_name} | Depth:␣
↪{depth}", unit="epoch") as pbar:
        for epoch in range(num_epochs):
            start_time = time.time()

            train_loss, train_acc = train_epoch_glove(model, train_loader,␣
↪optimizer, loss_function, device)
            train_losses.append(train_loss)
            train_accs.append(train_acc)
            val_acc, val_f1, val_loss = validate_epoch_glove(model, val_loader,␣
↪loss_function, device)
            val_losses.append(val_loss)
            val_accs.append(val_acc)
            val_f1s.append(val_f1)

            end_time = time.time()
            epoch_duration = end_time - start_time

            pbar.set_description(
                f"Optimizer: {optimizer_name} | Depth: {depth} | Epoch {epoch+1}/
↪{num_epochs} - "
                f"Train Loss: {train_loss:.4f}, Val Loss: {val_loss:.4f}, "
                f"Train ACC: {train_acc:.2%}, Val ACC: {val_acc:.2%}, "
                f"F1: {val_f1:.2f}, Time: {epoch_duration / 60:.2f} min"
            )
            pbar.update(1)

            wandb.log({
                'train_loss': train_loss,
                'val_loss': val_loss,
                'train_acc': train_acc,
                'val_acc': val_acc,
                'val_f1': val_f1,
            })

    wandb.finish()
```

```
 Training with optimizer: RMSprop | Depth: 1

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GloVe_GRU_BahdanauAttention(
  (embedding): Embedding(40002, 300)
  (gru): GRU(300, 300, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=600, out_features=300, bias=True)
    (v): Linear(in_features=300, out_features=1, bias=False)
  )
  (fc): Linear(in_features=600, out_features=9, bias=True)
  (dropout): Dropout(p=0.9, inplace=False)
)
Total trainable parameters: 13270209

Optimizer: RMSprop | Depth: 1 | Epoch 7/7 - Train Loss: 0.2242, Val Loss:
0.2720, Train ACC: 93.29%, Val ACC: 92.17%, F1: 0.92, Time: 0.81 min:
100%|| 7/7 [05:43<00:00, 49.09s/epoch]

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 Training with optimizer: RMSprop | Depth: 2

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GloVe_GRU_BahdanauAttention(
  (embedding): Embedding(40002, 300)
  (gru): GRU(300, 300, num_layers=2, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=600, out_features=300, bias=True)
    (v): Linear(in_features=300, out_features=1, bias=False)
  )
  (fc): Linear(in_features=600, out_features=9, bias=True)
  (dropout): Dropout(p=0.9, inplace=False)
)
Total trainable parameters: 14893809

Optimizer: RMSprop | Depth: 2 | Epoch 7/7 - Train Loss: 0.1988, Val Loss:
0.2774, Train ACC: 94.18%, Val ACC: 91.77%, F1: 0.92, Time: 1.70 min:
100%|| 7/7 [11:48<00:00, 101.19s/epoch]

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 Training with optimizer: RMSprop | Depth: 3

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GloVe_GRU_BahdanauAttention(
  (embedding): Embedding(40002, 300)
  (gru): GRU(300, 300, num_layers=3, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=600, out_features=300, bias=True)
    (v): Linear(in_features=300, out_features=1, bias=False)
  )
  (fc): Linear(in_features=600, out_features=9, bias=True)
  (dropout): Dropout(p=0.9, inplace=False)
)
Total trainable parameters: 16517409

Optimizer: RMSprop | Depth: 3 | Epoch 7/7 - Train Loss: 0.1936, Val Loss:
0.2914, Train ACC: 94.47%, Val ACC: 91.96%, F1: 0.92, Time: 2.45 min:
100%|| 7/7 [17:12<00:00, 147.55s/epoch]

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```

Depth value is set to 1.

2.1.4 Batch size value selection

[ ]:
```
num_epochs = 7
learning_rate = 9e-5
optimizer_class = optim.RMSprop
batch_sizes = [8, 16, 32, 64]
depth = 1

for BATCH_SIZE in batch_sizes:
    optimizer_name = "RMSprop"
    print(f"\n Training with optimizer: {optimizer_name} | Batch Size:␣
 ↪{BATCH_SIZE}")

    train_loader = DataLoader(train_dataset, batch_size=BATCH_SIZE, shuffle=True)
    val_loader = DataLoader(val_dataset, batch_size=BATCH_SIZE, shuffle=False)
    model = GloVe_GRU_BahdanauAttention(embedding_matrix=embedding_matrix,␣
 ↪hidden_dim=300, num_classes=NUM_CLASSES, num_layers=depth, dropout_prob=0.9).
 ↪to(device)
    optimizer = optimizer_class(model.parameters(), lr=learning_rate)
    wandb.init(
        project='Multi_Class_Batch_Tuning_gru_attention_glove300d',
        name=f"{optimizer_name}_batch{BATCH_SIZE}",
        config={
            'learning_rate': learning_rate,
            'num_epochs': num_epochs,
            'optimizer': optimizer_name,
            'model': 'GRU_Model',
            'embedding_dim': 300,
            'hidden_dim': 300,
            'dropout_prob': 0.9,
            'num_layers': depth,
            'batch_size': BATCH_SIZE
        }
    )

    print(model)
    num_params = count_parameters(model)
    print(f"Total trainable parameters: {num_params}")

    train_losses, val_losses = [], []
    train_accs, val_accs = [], []
    val_f1s = []

    with tqdm(total=num_epochs, desc=f"Optimizer: {optimizer_name} | Batch:␣
↪{BATCH_SIZE}", unit="epoch") as pbar:
        for epoch in range(num_epochs):
            start_time = time.time()

            train_loss, train_acc = train_epoch_glove(model, train_loader,␣
↪optimizer, loss_function, device)
            train_losses.append(train_loss)
            train_accs.append(train_acc)

            val_acc, val_f1, val_loss = validate_epoch_glove(model, val_loader,␣
↪loss_function, device)
            val_losses.append(val_loss)
            val_accs.append(val_acc)
            val_f1s.append(val_f1)

            end_time = time.time()
            epoch_duration = end_time - start_time

            pbar.set_description(
                f"Optimizer: {optimizer_name} | Batch: {BATCH_SIZE} | Epoch␣
↪{epoch+1}/{num_epochs} - "
```

```
                f"Train Loss: {train_loss:.4f}, Val Loss: {val_loss:.4f}, "
                f"Train ACC: {train_acc:.2%}, Val ACC: {val_acc:.2%}, "
                f"F1: {val_f1:.2f}, Time: {epoch_duration / 60:.2f} min"
            )
            pbar.update(1)

            wandb.log({
                'train_loss': train_loss,
                'val_loss': val_loss,
                'train_acc': train_acc,
                'val_acc': val_acc,
                'val_f1': val_f1,
            })

    wandb.finish()
```

```
 Training with optimizer: RMSprop | Batch Size: 8

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GloVe_GRU_BahdanauAttention(
  (embedding): Embedding(40002, 300)
  (gru): GRU(300, 300, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=600, out_features=300, bias=True)
    (v): Linear(in_features=300, out_features=1, bias=False)
  )
  (fc): Linear(in_features=600, out_features=9, bias=True)
  (dropout): Dropout(p=0.9, inplace=False)
)
Total trainable parameters: 13270209

Optimizer: RMSprop | Batch: 8 | Epoch 7/7 - Train Loss: 0.2344, Val Loss:
0.3327, Train ACC: 94.06%, Val ACC: 91.91%, F1: 0.92, Time: 1.74 min:
100%|| 7/7 [12:03<00:00, 103.31s/epoch]

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```

```
 Training with optimizer: RMSprop | Batch Size: 16

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GloVe_GRU_BahdanauAttention(
  (embedding): Embedding(40002, 300)
  (gru): GRU(300, 300, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=600, out_features=300, bias=True)
    (v): Linear(in_features=300, out_features=1, bias=False)
  )
  (fc): Linear(in_features=600, out_features=9, bias=True)
  (dropout): Dropout(p=0.9, inplace=False)
)
Total trainable parameters: 13270209

Optimizer: RMSprop | Batch: 16 | Epoch 7/7 - Train Loss: 0.2224, Val Loss:
0.2879, Train ACC: 93.59%, Val ACC: 91.67%, F1: 0.92, Time: 1.10 min:
100%|| 7/7 [07:40<00:00, 65.78s/epoch]

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 Training with optimizer: RMSprop | Batch Size: 32

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GloVe_GRU_BahdanauAttention(
  (embedding): Embedding(40002, 300)
  (gru): GRU(300, 300, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=600, out_features=300, bias=True)
    (v): Linear(in_features=300, out_features=1, bias=False)
  )
  (fc): Linear(in_features=600, out_features=9, bias=True)
  (dropout): Dropout(p=0.9, inplace=False)
)
Total trainable parameters: 13270209

Optimizer: RMSprop | Batch: 32 | Epoch 7/7 - Train Loss: 0.2311, Val Loss:
0.2679, Train ACC: 93.21%, Val ACC: 91.93%, F1: 0.92, Time: 0.80 min:
100%|| 7/7 [05:37<00:00, 48.25s/epoch]

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 Training with optimizer: RMSprop | Batch Size: 64

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GloVe_GRU_BahdanauAttention(
  (embedding): Embedding(40002, 300)
  (gru): GRU(300, 300, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=600, out_features=300, bias=True)
    (v): Linear(in_features=300, out_features=1, bias=False)
  )
  (fc): Linear(in_features=600, out_features=9, bias=True)
  (dropout): Dropout(p=0.9, inplace=False)
)
Total trainable parameters: 13270209

Optimizer: RMSprop | Batch: 64 | Epoch 7/7 - Train Loss: 0.2417, Val Loss:
0.2707, Train ACC: 92.87%, Val ACC: 91.96%, F1: 0.92, Time: 0.74 min:
100%|| 7/7 [05:13<00:00, 44.79s/epoch]

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```

Batch size value is set to 32.

#3. Test phase

```
[31]: def reinitialize_weights(model):
          """Reinitializes the model's weights by calling reset_parameters() for each␣
       ↪layer that supports it."""
          for layer in model.children():
              if hasattr(layer, 'reset_parameters'):
                  layer.reset_parameters()

      def plot_confusion_matrix(ax, y_true, y_pred, num_classes):
          """Plots a confusion matrix as a heatmap.

          Args:
              ax (matplotlib.axes.Axes): The axes on which to plot the confusion␣
       ↪matrix.
              y_true (list or array): The true class labels for the test set.
              y_pred (list or array): The predicted class labels for the test set.
              num_classes (int): The number of unique classes in the dataset.
          """
          cm = confusion_matrix(y_true, y_pred, labels=range(num_classes))
          sns.heatmap(cm, annot=True, fmt='g', cmap='Blues',␣
       ↪xticklabels=range(num_classes), yticklabels=range(num_classes), ax=ax)
          ax.set_xlabel('Predicted')
          ax.set_ylabel('True')
          ax.set_title('Confusion Matrix')

      def evaluate_and_analyze_glove(model, test_loader, device):
          model.eval()

          all_labels = []
          all_preds = []
          all_probs = []
          all_indices = []

          top_correct = []
          top_wrong = []

          with torch.no_grad():
              for idx, (inputs, labels, raw_text) in enumerate(test_loader):
                  inputs, labels = inputs.to(device), labels.to(device)

                  outputs = model(inputs)
                  probs = torch.softmax(outputs, dim=1)
```

```
            preds = torch.argmax(probs, dim=1)

            all_labels.extend(labels.cpu().numpy())
            all_preds.extend(preds.cpu().numpy())
            all_probs.extend(probs.cpu().numpy())
            all_indices.extend(range(len(labels)))

            correct_indices = (preds == labels).nonzero(as_tuple=True)[0]
            wrong_indices = (preds != labels).nonzero(as_tuple=True)[0]

            for correct_idx in correct_indices:
                top_correct.append({
                    'index': correct_idx.item(),
                    'true_label': labels[correct_idx].item(),
                    'predicted_label': preds[correct_idx].item(),
                    'probability': probs[correct_idx, preds[correct_idx]].cpu().
 ↪item(),
                    'text': raw_text[correct_idx.item()] if raw_text is not None␣
 ↪else None
                })

            for wrong_idx in wrong_indices:
                top_wrong.append({
                    'index': wrong_idx.item(),
                    'true_label': labels[wrong_idx].item(),
                    'predicted_label': preds[wrong_idx].item(),
                    'probability': probs[wrong_idx, preds[wrong_idx]].cpu().
 ↪item(),
                    'text': raw_text[wrong_idx.item()] if raw_text is not None␣
 ↪else None
                })

    df_correct = pd.DataFrame(top_correct)
    df_wrong = pd.DataFrame(top_wrong)

    class_report = classification_report(all_labels, all_preds, output_dict=True)
    df_results = pd.DataFrame(class_report).transpose()

    return df_results, df_correct, df_wrong, all_labels, all_probs

def evaluate_and_analyze_pubMedBert(model, test_loader, device):
    model.eval()
    all_labels = []
    all_preds = []
    all_probs = []
    all_indices = []
    all_texts = []
    wrong_samples = []

    with torch.no_grad():
        for batch_idx, batch in enumerate(test_loader):
            input_ids = batch['input_ids'].to(device)
            attention_mask = batch['attention_mask'].to(device)
            labels = batch['labels'].to(device)
            texts = batch['text']

            outputs = model(input_ids, attention_mask)
            probs = torch.softmax(outputs, dim=1)
            preds = torch.argmax(probs, dim=1)

            all_labels.extend(labels.cpu().numpy())
            all_preds.extend(preds.cpu().numpy())
            all_probs.extend(probs.cpu().numpy())
            all_indices.extend(range(batch_idx * test_loader.batch_size,␣
↪(batch_idx + 1) * test_loader.batch_size))
            all_texts.extend(texts)

            for idx, (pred, prob, label, text) in enumerate(zip(preds, probs,␣
↪labels, texts)):
                if pred != label:
                    wrong_samples.append({
                        "index": batch_idx * test_loader.batch_size + idx,
                        "true_label": label.item(),
                        "predicted_label": pred.item(),
                        "probability": prob[pred].item(),
                        "text": text
                    })

    class_stats = defaultdict(lambda: {'correct': 0, 'wrong': 0})
    for true_label, pred_label in zip(all_labels, all_preds):
        if true_label == pred_label:
            class_stats[true_label]['correct'] += 1
        else:
            class_stats[true_label]['wrong'] += 1

    class_results = []
    for cls in sorted(class_stats.keys()):
        total = class_stats[cls]['correct'] + class_stats[cls]['wrong']
        success_rate = (class_stats[cls]['correct'] / total) * 100 if total > 0␣
↪else 0
        failure_rate = (class_stats[cls]['wrong'] / total) * 100 if total > 0␣
↪else 0
        class_results.append({'class': cls, 'success_rate': success_rate,␣
↪'failure_rate': failure_rate})
```

```
    df_results = pd.DataFrame(class_results)
    df_wrong = pd.DataFrame(wrong_samples)

    correct_samples = []
    for idx, (pred, prob, label, text) in enumerate(zip(all_preds, all_probs,␣
↪all_labels, all_texts)):
        if pred == label:
            correct_samples.append({
                "index": idx,
                "true_label": label,
                "predicted_label": pred,
                "probability": prob[pred].item(),
                "text": text
            })

    df_correct = pd.DataFrame(correct_samples)

    return df_results, df_wrong, df_correct, all_labels, all_probs

def plot_wrong_distributions(wrong_indices, all_labels, all_preds, num_classes =␣
↪NUM_CLASSES):
    """Plots the distribution of wrong predictions for each class."""
    class_counts_wrong = defaultdict(int)

    for idx in wrong_indices:
        true_label = all_labels[idx]
        class_counts_wrong[true_label] += 1

    class_labels = sorted(class_counts_wrong.keys())
    counts = [class_counts_wrong[label] for label in class_labels]
    colors = sns.color_palette("husl", len(class_labels))

    class_names = [f"Class {label}" for label in class_labels]

    sns.set(style="whitegrid")
    plt.figure(figsize=(10, 8))
    plt.barh(class_names, counts, color=colors)
    plt.xlabel('Number of Wrong Predictions')
    plt.ylabel('Crop Disease Classes')
    plt.title('Distribution of Wrong Predictions for Each Class')

    for i, (count, name) in enumerate(zip(counts, class_names)):
        plt.text(count, i, str(count), ha='left', va='center')

    plt.show()
```

```
[ ]: models = {
         "GloVe_GRU_BahdanauAttention":␣
      ↪GloVe_GRU_BahdanauAttention(embedding_matrix=embedding_matrix, hidden_dim=300,␣
      ↪num_classes=NUM_CLASSES, num_layers=1, dropout_prob=0.9).to(device),
         "PubMedBERT_GRU_Attention": PubMedBERT_GRU_Attention(BERT_DIM,␣
      ↪HIDDEN_DIM,num_layers=1, dropout_prob=DROPOUT).to(device),
     }

     optimizers = {
         "GloVe_GRU_BahdanauAttention": optim.
      ↪RMSprop(models["GloVe_GRU_BahdanauAttention"].parameters(), lr=9e-5,␣
      ↪weight_decay = 1e-5),
         "PubMedBERT_GRU_Attention": optim.Adam(models["PubMedBERT_GRU_Attention"].
      ↪parameters(), lr=9e-5, weight_decay = 1e-5),
     }
```

```
[ ]: loss_function = torch.nn.CrossEntropyLoss()
     loss_gap_ratio = 1.25
     ax_accuracy_gap = 5
     num_epochs = 7

     model_metrics = {}

     for model_name, model in models.items():
         print(f"\nTraining {model_name} model...\n")
         print(model)
         num_params = count_parameters(model)
         print(f"Total trainable parameters: {num_params}")

         reinitialize_weights(model)
         optimizer = optimizers[model_name]
         scheduler = ReduceLROnPlateau(optimizer, mode='min', factor=0.5, patience=2,␣
      ↪verbose=True)

         if "PubMedBERT" in model_name:
             train_dataset = PubMedBERTBinaryDataset(X_train.tolist(), y_train,␣
      ↪tokenizer)
             val_dataset = PubMedBERTBinaryDataset(X_val.tolist(), y_val, tokenizer)
             test_dataset = PubMedBERTBinaryDataset(X_test.tolist(), y_test,␣
      ↪tokenizer)
         else:
             train_dataset = TextDataset(X_train_tensor, y_train,␣
      ↪raw_text_data=X_train)
             val_dataset = TextDataset(X_val_tensor, y_val, raw_text_data=X_val)
             test_dataset = TextDataset(X_test_tensor, y_test, raw_text_data=X_test)
```

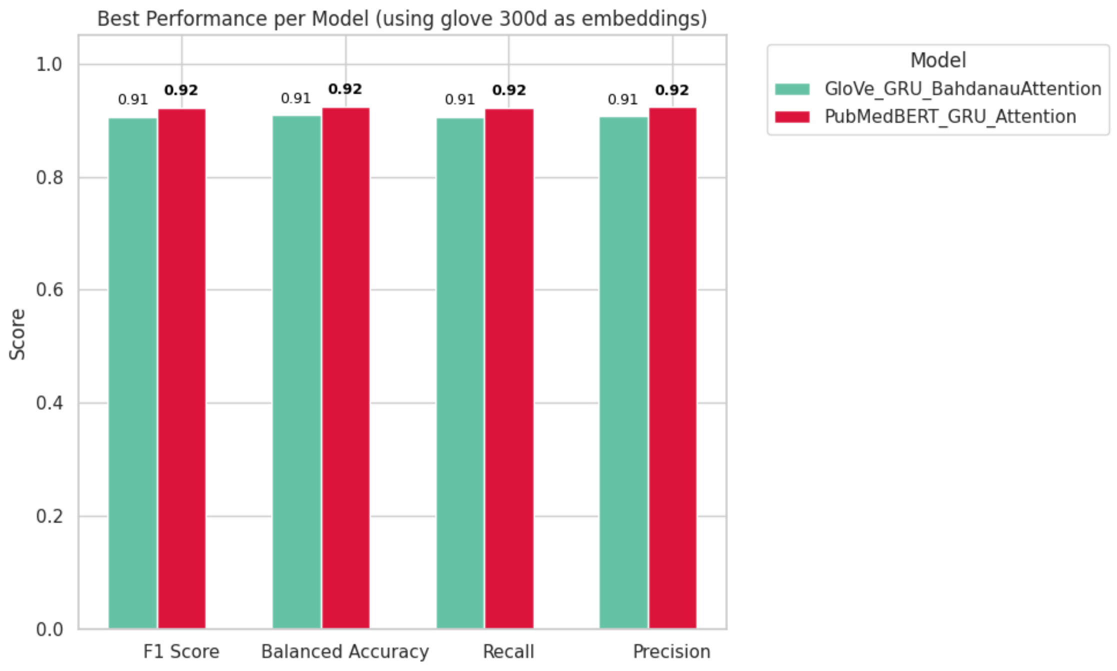
```
    train_loader = DataLoader(train_dataset, batch_size=BATCH_SIZE, shuffle=True)
    val_loader = DataLoader(val_dataset, batch_size=BATCH_SIZE, shuffle=False)
    test_loader = DataLoader(test_dataset, batch_size=BATCH_SIZE, shuffle=False)
    combined_dataset = ConcatDataset([train_dataset, val_dataset])
    combined_loader = DataLoader(combined_dataset, batch_size=BATCH_SIZE,␣
↪shuffle=True)

    wandb.init(
        project='Multi-Class-Models-Train-Test-PubeMedBERT-Glove300d-Attention',
        name=f"{model_name}_Training",
        config={
            'learning_rate': 9e-5,
            'num_epochs': num_epochs,
            'num_layers': 1
        }
    )

    train_losses, test_losses = [], []
    train_accuracies, test_accuracies = [], []
    test_f1s, test_balanced_accs, test_recalls, test_precisions = [], [], [], []

    saved_once = False
    with tqdm(total=num_epochs, desc=f"Training {model_name}", unit="epoch") as␣
↪pbar:
        for epoch in range(num_epochs):
            start_time = time.time()

            if "PubMedBERT" in model_name:
                train_loss, train_acc = train_model(model, combined_loader,␣
↪optimizer, loss_function, device)
                test_loss, test_acc, test_f1, test_balanced_acc, test_recall,␣
↪test_precision = test_model(
                    model, test_loader, loss_function, device)
            else:
                train_loss, train_acc = train_epoch_glove(model,␣
↪combined_loader, optimizer, loss_function, device)
                test_loss, test_acc, test_f1, test_balanced_acc, test_recall,␣
↪test_precision = test_epoch_glove(
                    model, test_loader, loss_function, device)

            train_losses.append(train_loss)
            test_losses.append(test_loss)
            train_accuracies.append(train_acc)
            test_accuracies.append(test_acc)
            test_f1s.append(test_f1)
            test_balanced_accs.append(test_balanced_acc)
            test_recalls.append(test_recall)
            test_precisions.append(test_precision)

            wandb.log({
                "train_loss": train_loss,
                "test_loss": test_loss,
                "train_acc": train_acc,
                "test_acc": test_acc,
                "test_f1": test_f1,
                "test_balanced_acc": test_balanced_acc,
                "test_recall": test_recall,
                "test_precision": test_precision
            })

            if (test_loss > train_loss * loss_gap_ratio or train_acc - test_acc␣
↪> ax_accuracy_gap / 100) and not saved_once:
                torch.save(model.state_dict(), f"{model_name}_early_stop.pth")
                saved_once = True
                break

            if epoch == num_epochs - 1 and not saved_once:
                torch.save(model.state_dict(), f"{model_name}_final.pth")

            pbar.set_description(
                f"{model_name} Epoch {epoch+1}/{num_epochs} - Train Loss:␣
↪{train_loss:.4f}, Test Loss: {test_loss:.4f}, "
                f"Train Acc: {train_acc:.2%}, Test Acc: {test_acc:.2%}, Test F1:␣
↪{test_f1:.2%}, "
                f"Test Balanced Acc: {test_balanced_acc:.2%}, Test Recall:␣
↪{test_recall:.2%}, Test Precision: {test_precision:.2%}, "
                f"Time: {(time.time() - start_time) / 60:.2f} min"
            )
            pbar.update(1)

        epoch_table = wandb.Table(columns=["Epoch", "Train Loss", "Test Loss",␣
↪"Train Acc", "Test Acc", "F1", "Balanced Acc", "Recall", "Precision"])
        for epoch in range(len(train_losses)):
            epoch_table.add_data(epoch + 1, train_losses[epoch],␣
↪test_losses[epoch], train_accuracies[epoch],
                                 test_accuracies[epoch], test_f1s[epoch],␣
↪test_balanced_accs[epoch],
                                 test_recalls[epoch], test_precisions[epoch])
        wandb.log({f"{model_name}_Metrics_Table": epoch_table})

        wandb.log({
            'train_loss_over_epochs': wandb.plot.line_series(
                xs=list(range(1, num_epochs+1)),
                ys=[train_losses, test_losses],
                keys=['Train Loss', 'Test Loss'],
                title='Loss Over Epochs',
                xname='Epoch'
            ),
            'train_acc_over_epochs': wandb.plot.line_series(
                xs=list(range(1, num_epochs+1)),
                ys=[train_accuracies, test_accuracies],
                keys=['Train Accuracy', 'Test Accuracy'],
                title='Accuracy Over Epochs',
                xname='Epoch'
            ),
            'test_f1_over_epochs': wandb.plot.line_series(
                xs=list(range(1, num_epochs+1)),
                ys=[test_f1s],
                keys=['Test F1 Score'],
                title='Test F1 Score Over Epochs',
                xname='Epoch'
            )
        })

        model_metrics[model_name] = {
            "train_losses": train_losses,
            "test_losses": test_losses,
            "train_accuracies": train_accuracies,
            "test_accuracies": test_accuracies,
            "test_f1s": test_f1s,
            "test_balanced_accs": test_balanced_accs,
            "test_recalls": test_recalls,
            "test_precisions": test_precisions
        }
```

```
Training GloVe_GRU_BahdanauAttention model...

GloVe_GRU_BahdanauAttention(
  (embedding): Embedding(40002, 300)
  (gru): GRU(300, 300, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=600, out_features=300, bias=True)
    (v): Linear(in_features=300, out_features=1, bias=False)
  )
  (fc): Linear(in_features=600, out_features=9, bias=True)
  (dropout): Dropout(p=0.9, inplace=False)
)
Total trainable parameters: 13270209
```

```
<ipython-input-15-811d6649565c>:44: UserWarning: To copy construct from a
tensor, it is recommended to use sourceTensor.clone().detach() or
sourceTensor.clone().detach().requires_grad_(True), rather than
torch.tensor(sourceTensor).
  self.X = torch.tensor(X_data, dtype=torch.long)
wandb: Using wandb-core as the SDK backend.  Please refer to
https://wandb.me/wandb-core for more information.

<IPython.core.display.Javascript object>

wandb: Logging into wandb.ai. (Learn how to deploy a W&B server
locally: https://wandb.me/wandb-server)
wandb: You can find your API key in your browser here:
https://wandb.ai/authorize
wandb: Paste an API key from your profile and hit enter:

 ··········

wandb: WARNING If you're specifying your api key in code,
ensure this code is not shared publicly.
wandb: WARNING Consider setting the WANDB_API_KEY
environment variable, or running `wandb login` from the command line.
wandb: No netrc file found, creating one.
wandb: Appending key for api.wandb.ai to your netrc file:
/root/.netrc
wandb: Currently logged in as: wilfried-mvomoeto
(wilfried-mvomoeto-university-of-li-ge) to
https://api.wandb.ai. Use `wandb login --relogin` to force
relogin

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

GloVe_GRU_BahdanauAttention Epoch 7/7 - Train Loss: 0.2639, Test Loss: 0.2997,
Train Acc: 91.91%, Test Acc: 90.63%, Test F1: 90.64%, Test Balanced Acc: 90.86%,
Test Recall: 90.63%, Test Precision: 90.67%, Time: 1.01 min: 100%||
7/7 [07:25<00:00, 63.63s/epoch]


Training PubMedBERT_GRU_Attention model...

PubMedBERT_GRU_Attention(
  (gru): GRU(768, 256, batch_first=True, bidirectional=True)
  (attention): BahdanauAttention(
    (W): Linear(in_features=512, out_features=256, bias=True)
    (v): Linear(in_features=256, out_features=1, bias=False)
  )
  (fc): Linear(in_features=512, out_features=9, bias=True)
  (dropout): Dropout(p=0.6, inplace=False)
)
Total trainable parameters: 1712137

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

PubMedBERT_GRU_Attention Epoch 6/7 - Train Loss: 0.2049, Test Loss: 0.2507,
Train Acc: 93.50%, Test Acc: 92.00%, Test F1: 92.01%, Test Balanced Acc: 92.28%,
Test Recall: 92.00%, Test Precision: 92.06%, Time: 15.78 min:  86%| |
6/7 [1:50:31<18:25, 1105.23s/epoch]
```

[ ]:
```
summary_metrics = {
    "Model": [],
    "F1 Score": [],
    "Balanced Accuracy": [],
    "Recall": [],
    "Precision": []
}

for model_name, metrics in model_metrics.items():
    summary_metrics["Model"].append(model_name)
    summary_metrics["F1 Score"].append(max(metrics["test_f1s"]))
    summary_metrics["Balanced Accuracy"].
 ↪append(max(metrics["test_balanced_accs"]))
    summary_metrics["Recall"].append(max(metrics["test_recalls"]))
    summary_metrics["Precision"].append(max(metrics["test_precisions"]))

df_summary = pd.DataFrame(summary_metrics)
df_melted = df_summary.melt(id_vars="Model", var_name="Metric",␣
 ↪value_name="Score")

sns.set(style="whitegrid")
fig, ax = plt.subplots(figsize=(10, 6))
```

```
models = df_summary["Model"].tolist()
palette = sns.color_palette("Set2", len(models))

for i, metric in enumerate(df_melted["Metric"].unique()):
    data = df_melted[df_melted["Metric"] == metric]
    max_score = data["Score"].max()

    for j, (index, row) in enumerate(data.iterrows()):
        color = "crimson" if row["Score"] == max_score else palette[models.
↪index(row["Model"])]
        bar = ax.bar(
            x=i - 0.3 + j * (0.6 / len(models)),
            height=row["Score"],
            width=0.6 / len(models),
            color=color,
            label=row["Model"] if i == 0 else "",
        )
        ax.text(
            x=bar[0].get_x() + bar[0].get_width() / 2,
            y=row["Score"] + 0.015,
            s=f"{row['Score']:.2f}",
            ha='center',
            va='bottom',
            fontsize=9,
            color='black',
            fontweight='bold' if row["Score"] == max_score else 'normal'
        )

ax.set_xticks(range(len(df_melted["Metric"].unique())))
ax.set_xticklabels(df_melted["Metric"].unique())
ax.set_ylim(0, 1.05)
ax.set_ylabel("Score")
ax.set_title("Best Performance per Model (using glove 300d as embeddings)")
ax.grid(True, axis='y')

handles, labels = ax.get_legend_handles_labels()
by_label = dict(zip(labels, handles))
ax.legend(by_label.values(), by_label.keys(), title="Model", bbox_to_anchor=(1.
↪05, 1), loc="upper left")

plt.tight_layout()
plt.savefig("best_model_performance_comparison_all_values_glove300d.png")
plt.show()
```



The PubMedBERT-based model with Bidirectional GRU and Bahdanau Attention consistently outperforms the GloVe-based model with Bidirectional GRU and Bahdanau Attention across all key metrics, though by a small margin of 0.01.

This performance gain, while subtle, demonstrates that contextual embeddings like PubMedBERT provide a more nuanced and contextual understanding of biomedical text compared to traditional word embeddings like GloVe.

Furthermore, the consistency across F1 Score, Precision, Recall, and Balanced Accuracy suggests that the PubMedBERT-based model with Bidirectional GRU and Bahdanau Attention delivers more stable and generalizable predictions, which is especially valuable when dealing with class-imbalanced biomedical datasets

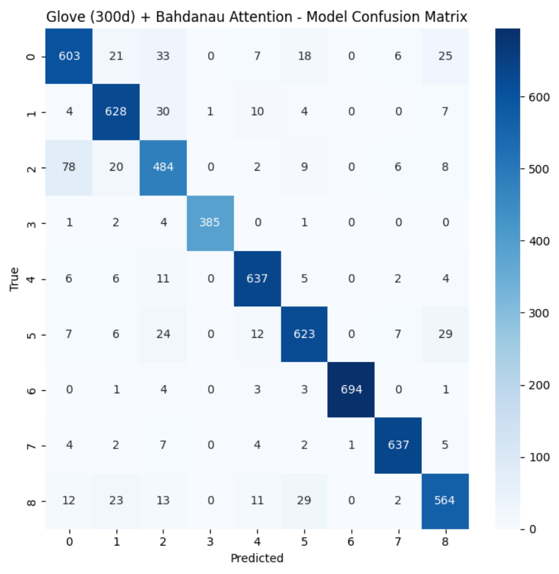
[ ]:
```
with open("model_metrics.pkl", "wb") as f:
    pickle.dump(model_metrics, f)

with open("model_metrics.pkl", "rb") as f:
    model_metrics = pickle.load(f)
```

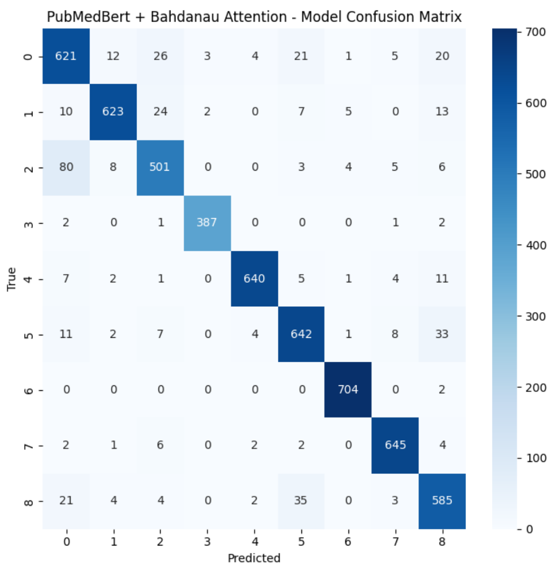
[32]:
```
test_dataset_pubMed = PubMedBERTBinaryDataset(X_test.tolist(), y_test, tokenizer)
test_dataset_glove = TextDataset(X_test_tensor, y_test, raw_text_data=X_test)

test_loader_pubMed = DataLoader(test_dataset_pubMed, batch_size=BATCH_SIZE,␣
↪shuffle=False)
```

```
test_loader_glove = DataLoader(test_dataset_glove, batch_size=BATCH_SIZE,␣
↪shuffle=False)

model_glove = GloVe_GRU_BahdanauAttention(embedding_matrix=embedding_matrix,␣
↪hidden_dim=300, num_classes=NUM_CLASSES, num_layers=1, dropout_prob=0.9).
↪to(device)
model_glove.load_state_dict(torch.load("/content/drive/MyDrive/
↪GloVe_GRU_BahdanauAttention_final.pth"))

model_pubMedBert = PubMedBERT_GRU_Attention(BERT_DIM, HIDDEN_DIM, num_layers=1,␣
↪dropout_prob=DROPOUT).to(device)
model_pubMedBert.load_state_dict(torch.load("/content/drive/MyDrive/
↪PubMedBERT_GRU_Attention_early_stop.pth"))

df_results_glove, df_correct_glove, df_wrong_glove, all_labels_glove,␣
↪all_probs_glove = evaluate_and_analyze_glove(model_glove, test_loader_glove,␣
↪device)
df_results_pubMedBert, df_wrong_pubMedBert, df_correct_pubMedBert,␣
↪all_labels_pubMedBert, all_probs_pubMedBert =␣
↪evaluate_and_analyze_pubMedBert(model_pubMedBert, test_loader_pubMed, device)
```

```
<ipython-input-16-811d6649565c>:44: UserWarning: To copy construct from a
tensor, it is recommended to use sourceTensor.clone().detach() or
sourceTensor.clone().detach().requires_grad_(True), rather than
torch.tensor(sourceTensor).
  self.X = torch.tensor(X_data, dtype=torch.long)
```

[33]:
```
all_preds_glove = np.argmax(np.array(all_probs_glove), axis=1)
all_preds_pubMedBert = np.argmax(np.array(all_probs_pubMedBert), axis=1)

fig, axes = plt.subplots(1, 2, figsize=(14, 7))

plot_confusion_matrix(axes[0], all_labels_glove, all_preds_glove, NUM_CLASSES)
axes[0].set_title("Glove (300d) + Bahdanau Attention - Model Confusion Matrix")

plot_confusion_matrix(axes[1], all_labels_pubMedBert, all_preds_pubMedBert,␣
↪NUM_CLASSES)
axes[1].set_title("PubMedBert + Bahdanau Attention - Model Confusion Matrix")

plt.tight_layout()
plt.show()
```





0.2.1 Confusion Matrix Comparison Summary

This section compares the performance of two models using confusion matrices:

- **Model 1:** GloVe (300d) as word embeddings + Bidirectional GRU + Bahdanau Attention

- **Model 2:** PubMedBert as contextual embeddings + Bidirectional GRU + Bahdanau Attention

---

Key Observations

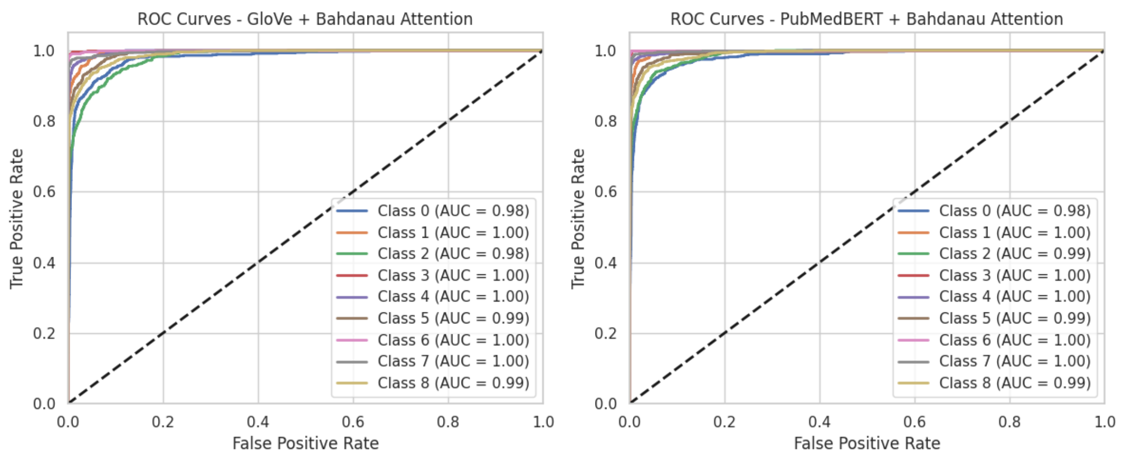
- **Overall Accuracy:**
  - The model using contextual embeddings (**PubMedBert**) outperforms the one using word embeddings (**GloVe**) in most classes, demonstrating better generalization and fewer misclassifications.
- **Diagonal Strength (Correct Predictions):**
  - **PubMedBert** shows higher or equal correct predictions in critical classes like **0, 5, and 8**.
  - Both models perform nearly identically on **class 3** and exceptionally well on **class 6**, with minimal misclassifications.
- **Common Misclassifications:**
  - **GloVe-based model** exhibits higher confusion in **class 2** and **class 8**, misclassifying several samples into other classes.
  - **PubMedBert-based model** also makes some misclassifications (notably between classes **0, 2, and 5**) but at a reduced rate.

Conclusion

PubMedBert + Bidirectional GRU + Bahdanau Attention demonstrates superior performance over the **GloVe-based bidirectional GRU model**, particularly in biomedical class predictions. It consistently shows **lower off-diagonal error rates**, making it more robust and reliable for downstream tasks.

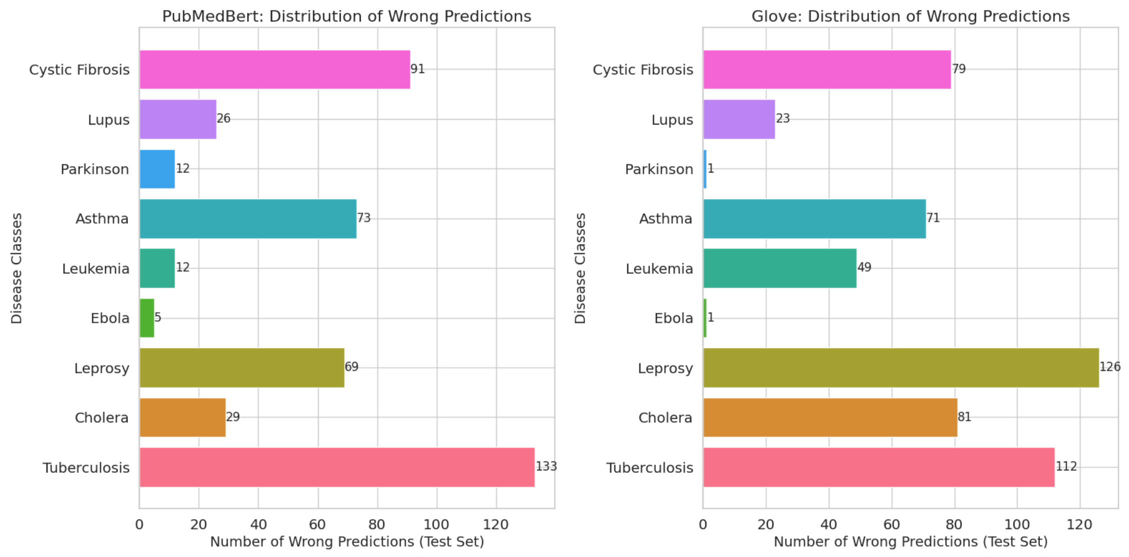
[35]:
```
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.metrics import roc_curve, auc
from sklearn.preprocessing import label_binarize

n_classes = 9
class_names = [f'Class {i}' for i in range(n_classes)]

y_true_glove = np.array(all_labels_glove)
y_score_glove = np.array(all_probs_glove)
y_true_bin_glove = label_binarize(y_true_glove, classes=list(range(n_classes)))

y_true_pubMedBert = np.array(all_labels_pubMedBert)
y_score_pubMedBert = np.array(all_probs_pubMedBert)
y_true_bin_pubMedBert = label_binarize(y_true_pubMedBert,␣
↪classes=list(range(n_classes)))

if y_score_glove.ndim != 2 or y_score_glove.shape[1] != n_classes:
    raise ValueError("y_score_glove must be an array with shape (n_samples,␣
↪n_classes) containing probabilities for each class.")
if y_score_pubMedBert.ndim != 2 or y_score_pubMedBert.shape[1] != n_classes:
    raise ValueError("y_score_pubMedBert must be an array with shape (n_samples,␣
↪n_classes) containing probabilities for each class.")

fpr_glove, tpr_glove, roc_auc_glove = {}, {}, {}
fpr_pubMedBert, tpr_pubMedBert, roc_auc_pubMedBert = {}, {}, {}

for i in range(n_classes):
    fpr_glove[i], tpr_glove[i], _ = roc_curve(y_true_bin_glove[:, i],␣
↪y_score_glove[:, i])
    roc_auc_glove[i] = auc(fpr_glove[i], tpr_glove[i])

    fpr_pubMedBert[i], tpr_pubMedBert[i], _ = roc_curve(y_true_bin_pubMedBert[:,␣
↪i], y_score_pubMedBert[:, i])
    roc_auc_pubMedBert[i] = auc(fpr_pubMedBert[i], tpr_pubMedBert[i])
```

[38]:
```
sns.set(style="whitegrid")
fig, axes = plt.subplots(1, 2, figsize=(12, 5))

for i in range(n_classes):
    axes[0].plot(fpr_glove[i], tpr_glove[i], lw=2, label=f'{class_names[i]} (AUC␣
↪= {roc_auc_glove[i]:.2f})')

axes[0].plot([0, 1], [0, 1], 'k--', lw=2)
axes[0].set_xlim([0.0, 1.0])
axes[0].set_ylim([0.0, 1.05])
axes[0].set_xlabel('False Positive Rate')
axes[0].set_ylabel('True Positive Rate')
axes[0].set_title('ROC Curves - GloVe + Bahdanau Attention')
axes[0].legend(loc='lower right')
axes[0].grid(True)

for i in range(n_classes):
    axes[1].plot(fpr_pubMedBert[i], tpr_pubMedBert[i], lw=2,␣
↪label=f'{class_names[i]} (AUC = {roc_auc_pubMedBert[i]:.2f})')

axes[1].plot([0, 1], [0, 1], 'k--', lw=2)
axes[1].set_xlim([0.0, 1.0])
axes[1].set_ylim([0.0, 1.05])
axes[1].set_xlabel('False Positive Rate')
axes[1].set_ylabel('True Positive Rate')
axes[1].set_title('ROC Curves - PubMedBERT + Bahdanau Attention')
axes[1].legend(loc='lower right')
axes[1].grid(True)

plt.tight_layout()
plt.show()
```



```
[ ]: class_names_dict = {
         0: 'Tuberculosis',
         1: 'Cholera',
    2: 'Leprosy',
    3: 'Ebola',
    4: 'Leukemia',
    5: 'Asthma',
    6: 'Parkinson',
    7: 'Lupus',
    8: 'Cystic Fibrosis'
}

wrong_df_pubMedBert = pd.DataFrame({'predictions': all_preds_pubMedBert,␣
 ↪'labels': all_labels_pubMedBert})
wrong_df_pubMedBert['wrong'] = wrong_df_pubMedBert['predictions'] !=␣
 ↪wrong_df_pubMedBert['labels']

wrong_df_glove = pd.DataFrame({'predictions': all_preds_glove, 'labels':␣
 ↪all_labels_glove})
wrong_df_glove['wrong'] = wrong_df_glove['predictions'] !=␣
 ↪wrong_df_glove['labels']

def get_wrong_counts(df):
    wrong_class_counts = defaultdict(int)
    for _, row in df.iterrows():
        if row['wrong']:
            wrong_class_counts[row['predictions']] += 1
    wrong_class_labels = sorted(wrong_class_counts.keys())
    wrong_counts = [wrong_class_counts[label] for label in wrong_class_labels]
    return wrong_class_labels, wrong_counts

wrong_class_labels_pubMedBert, wrong_counts_pubMedBert =␣
 ↪get_wrong_counts(wrong_df_pubMedBert)
wrong_class_labels_glove, wrong_counts_glove = get_wrong_counts(wrong_df_glove)


sns.set(style="whitegrid", palette="muted", font_scale=1.3)
fig, axes = plt.subplots(1, 2, figsize=(16, 8))

wrong_colors_pubMedBert = sns.color_palette("husl",␣
 ↪len(wrong_class_labels_pubMedBert))
class_names_pubMedBert = [class_names_dict[label] for label in␣
 ↪wrong_class_labels_pubMedBert]
axes[0].barh(class_names_pubMedBert, wrong_counts_pubMedBert,␣
 ↪color=wrong_colors_pubMedBert)
axes[0].set_xlabel('Number of Wrong Predictions (Test Set)', fontsize=14)
axes[0].set_ylabel('Disease Classes', fontsize=14)
axes[0].set_title('PubMedBert: Distribution of Wrong Predictions', fontsize=16)
```

```
for i, (count, name) in enumerate(zip(wrong_counts_pubMedBert,␣
↪class_names_pubMedBert)):
    axes[0].text(count, i, str(count), ha='left', va='center', fontsize=12)

wrong_colors_glove = sns.color_palette("husl", len(wrong_class_labels_glove))
class_names_glove = [class_names_dict[label] for label in␣
↪wrong_class_labels_glove]
axes[1].barh(class_names_glove, wrong_counts_glove, color=wrong_colors_glove)
axes[1].set_xlabel('Number of Wrong Predictions (Test Set)', fontsize=14)
axes[1].set_ylabel('Disease Classes', fontsize=14)
axes[1].set_title('Glove: Distribution of Wrong Predictions', fontsize=16)
for i, (count, name) in enumerate(zip(wrong_counts_glove, class_names_glove)):
    axes[1].text(count, i, str(count), ha='left', va='center', fontsize=12)

plt.tight_layout()
plt.show()
```



Summary

Using PubMedBert enables to achieve lower misclassification rates in 5 out of 9 disease classes, especially for:

Leprosy: 45% fewer wrong predictions

Cholera: 64% fewer wrong predictions

Leukemia: 75% fewer wrong predictions

Using GloVe enables to perform slightly better in Parkinson, Ebola, and Tuberculosis.

Tuberculosis remains the most challenging class for both models, especially PubMedBert.

Voici la table mise à jour avec les meilleures valeurs de chaque colonne mises en **gras** :

---

1 Model Performance Comparison

Model	**Input Type**	**Accuracy**	**Balanced Accuracy**	**F1 Score**	**Recall**	**Precision**
GRU	No embeddings	87.74%	88.00%	87.78%	87.74%	88.00%
LSTM	No embeddings	88.13%	88.46%	88.36%	88.13%	88.88%
CNN + GRU	No embeddings	86.77%	87.09%	87.11%	86.77%	88.35%
CNN + LSTM	No embeddings	88.13%	88.40%	88.36%	88.13%	89.34%
GRU	GloVe (300d)	**92.17%**	**92.36%**	**92.15%**	**92.17%**	**92.21%**
LSTM	GloVe (300d)	88.34%	88.82%	88.41%	88.34%	89.07%
CNN + GRU	GloVe (300d)	89.70%	89.86%	89.65%	89.70%	89.74%
CNN + LSTM	GloVe (300d)	88.88%	89.13%	88.97%	88.88%	89.60%
Bidirectional GRU + Bahdanau Attention	**PubMedBERT**	**92.00%**	**92.28%**	**92.01%**	**92.00%**	**92.06%**
Bidirectional GRU + Bahdanau Attention	GloVe (300d)	**90.63%**	**90.86%**	**90.64%**	**90.63%**	**90.67%**

Given the imbalance in the dataset, we are now tackling this issue by implementing techniques such as SMOTE, weighted training, and ADASYN. We will evaluate their impact by measuring improvements in model performance and the balance of the data distribution.