BeFree-3class-gru

September 18, 2024

1 Evaluation using the BeFree corpus

1.0.1 GAD dataset

To obtain a large benchmark of Gene Disease Associations along with associated sentences from literature, we used the corpus generated by BeFree system based on Genetic Association Database (GAD)

2 —————

3 imports

```
[1]: import tensorflow as tf
     import keras
     from keras.models import load model
     from keras.callbacks import ModelCheckpoint, EarlyStopping
     from keras_tqdm import TQDMNotebookCallback
     import numpy as np
     np.random.seed(1337)
     from keras_tqdm import TQDMNotebookCallback
     import nltk
     import xml.etree.ElementTree as ET
     import pandas as pd
     import os
     import string
     from nltk.tokenize import TreebankWordTokenizer
     from numpy.random import random_sample
     import re
     import pickle
     from sklearn.metrics import accuracy_score
     from sklearn.metrics import classification_report
     from keras.layers import Embedding, Flatten, LSTM, GRU
     from keras.layers.convolutional import Conv2D, MaxPooling2D
     from tensorflow.keras.utils import to_categorical
     from tensorflow.keras.models import Sequential, Model
```

```
from keras.layers import Dense, Dropout, Activation, Input,
merge,Conv1D,MaxPooling1D,GlobalMaxPooling1D,Convolution1D
from keras import regularizers
from sklearn.metrics import precision_recall_fscore_support
from sklearn.model_selection import StratifiedKFold
import matplotlib.pyplot as plt
from keras.layers import Concatenate, concatenate
from keras import backend as K
from keras.layers import multiply
from keras.layers import merge
from keras.layers.core import *
from keras.layers.recurrent import LSTM
from keras.models import *
random_seed=1337
```

Using TensorFlow backend.

3.0.1 Define Callback functions to generate Measures

```
from keras import backend as K

def f1(y_true, y_pred):
    def recall(y_true, y_pred):
        true_positives = K.sum(K.round(K.clip(y_true * y_pred, 0, 1)))
        possible_positives = K.sum(K.round(K.clip(y_true, 0, 1)))
        recall = true_positives / (possible_positives + K.epsilon())
        return recall

def precision(y_true, y_pred):
        true_positives = K.sum(K.round(K.clip(y_true * y_pred, 0, 1)))
        predicted_positives = K.sum(K.round(K.clip(y_pred, 0, 1)))
        precision = true_positives / (predicted_positives + K.epsilon())
        return precision
    precision = precision(y_true, y_pred)
    recall = recall(y_true, y_pred)
    return 2*((precision*recall)/(precision+recall+K.epsilon()))
```

4 Experiments to reproduce the results of Table 7

4.0.1 Evaluation results for multi-class classification

4.0.2 Load Prerocssed Data

```
[3]: with open('../data/pickles/befree_3class_crawl-300d-2M.pickle', 'rb') as handle:
    gene_id_list = pickle.load(handle)
    gene_symbol_list = pickle.load(handle)
    disease_id_list = pickle.load(handle)
    X_train = pickle.load(handle)
```

```
distance1_vectors = pickle.load(handle)
  distance2_vectors = pickle.load(handle)
  Y_train = pickle.load(handle)
  word_list = pickle.load(handle)
  word_vectors = pickle.load(handle)
  word_dict = pickle.load(handle)
  distance1_dict = pickle.load(handle)
  distance2_dict = pickle.load(handle)
  label_dict = pickle.load(handle)
  MAX_SEQUENCE_LENGTH = pickle.load(handle)
  print ("word_vectors",len(word_vectors))
```

word_vectors 6766

4.0.3 Create Position Embedding Vectors

[4]: (5330, 81, 20)

4.0.4 Prepare Word Embedding Layer

```
[5]: EMBEDDING_DIM=word_vectors.shape[1]
print("EMBEDDING_DIM=",EMBEDDING_DIM)
embedding_matrix=word_vectors

def create_embedding_layer(12_reg=0.01,use_pretrained=True,is_trainable=False):
    if use_pretrained:
```

```
return Embedding(len(word_dict)

,EMBEDDING_DIM,weights=[embedding_matrix],input_length=MAX_SEQUENCE_LENGTH,trainable=is_tra
.12(12_reg))

else:
    return Embedding(len(word_dict)
.,EMBEDDING_DIM,input_length=MAX_SEQUENCE_LENGTH)
```

EMBEDDING DIM= 300

4.0.5 Prepare Attention Mechanism

4.0.6 Create the Model

```
x = MaxPooling1D(3)(x)
         x = Dropout(0.1)(x)
         conv_sequence_w5=GlobalMaxPooling1D()(x) #x = Flatten()(x)
         x = Conv1D(64, 3, activation='relu')(embedded_sequences)
        x = MaxPooling1D(3)(x)
         x = Dropout(0.1)(x)
         conv_sequence_w4=GlobalMaxPooling1D()(x) #x = Flatten()(x)
         x = Conv1D(128, 3, activation='relu')(embedded_sequences)
         x = MaxPooling1D(3)(x)
         x = Dropout(0.1)(x)
         conv_sequence_w3=GlobalMaxPooling1D()(x) #x = Flatten()(x)
         forward = GRU(100, recurrent_dropout=0.
      →05,return_sequences=True)(embedded_sequences)
         backward = GRU(100, go backwards=True, recurrent dropout=0.
      →05, return_sequences=True) (embedded_sequences)
         attention_forward=attentionNew(forward)
         attention_backward=attentionNew(backward)
         lstm_sequence = concatenate([attention_forward,attention_backward])
         lstm_sequence = Flatten()(lstm_sequence)
         merge =
      -concatenate([conv_sequence_w5,conv_sequence_w4,conv_sequence_w3,1stm_sequence])
         x = Dense(64, activation='relu', kernel regularizer=regularizers.12(0.
      \hookrightarrow1))(merge)
         x = Dropout(0.1)(x)
         preds = Dense(3, activation='softmax')(x)
         model = Model(inputs=[sequence_input,__

¬pos_embedd_1,pos_embedd_2],outputs=preds)
         opt=tf.keras.optimizers.Adam()
         model.
      acompile(loss='categorical_crossentropy',optimizer=opt,metrics=['acc',f1])
         return model
[8]: model = build_model()
     model.summary()
    Model: "model_1"
```

Layer (type)	Output Shape	Param #	Connected to
input_1 (InputLayer)			
embedding_1 (Embedding)		2029800	input_1[0][0]
input_2 (InputLayer)	(None, 81, 20)	0	
	(None, 81, 20)	0	
concatenate_1 (Concatenate) embedding_1[0][0]			
			input_2[0][0] input_3[0][0]
gru_1 (GRU) concatenate_1[0][0]	(None, 81, 100)		
gru_2 (GRU) concatenate_1[0][0]	(None, 81, 100)		
lambda_1 (Lambda)	(None, 81, 100)		
lambda_3 (Lambda)	(None, 81, 100)		
permute_1 (Permute)	(None, 100, 81)		lambda_1[0][0]
permute_3 (Permute)	(None, 100, 81)	0	
dense_1 (Dense)	(None, 100, 81)		=
dense_2 (Dense)	(None, 100, 81)	6642	permute_3[0][0]
permute_2 (Permute)	(None, 81, 100)		

permute_4 (Permute)	(None, 81, 100)	0	dense_2[0][0]
conv1d_1 (Conv1D) concatenate_1[0][0]	(None, 77, 32)	54432	
conv1d_2 (Conv1D) concatenate_1[0][0]	(None, 79, 64)	65344	
conv1d_3 (Conv1D) concatenate_1[0][0]	(None, 79, 128)	130688	
multiply_1 (Multiply)	(None, 81, 100)	0	lambda_1[0][0] permute_2[0][0]
multiply_2 (Multiply)	(None, 81, 100)	0	lambda_3[0][0] permute_4[0][0]
max_pooling1d_1 (MaxPooling1D)		0	conv1d_1[0][0]
max_pooling1d_2 (MaxPooling1D)			conv1d_2[0][0]
max_pooling1d_3 (MaxPooling1D)	(None, 26, 128)	0	conv1d_3[0][0]
lambda_2 (Lambda) multiply_1[0][0]	(None, 81, 100)	0	
lambda_4 (Lambda) multiply_2[0][0]	(None, 81, 100)	0	
dropout_1 (Dropout) max_pooling1d_1[0][0]	(None, 25, 32)	0	
dropout_2 (Dropout) max_pooling1d_2[0][0]	(None, 26, 64)	0	

dropout_3 (Dropout) max_pooling1d_3[0][0]	(None,	26, 128)	0	
concatenate_2 (Concatenate)	(None,	81, 200)	0	lambda_2[0][0] lambda_4[0][0]
global_max_pooling1d_1 (GlobalM			0	dropout_1[0][0]
global_max_pooling1d_2 (GlobalM			0	dropout_2[0][0]
global_max_pooling1d_3 (GlobalM	(None,	128)	0	dropout_3[0][0]
flatten_1 (Flatten) concatenate_2[0][0]	(None,	16200)	0	
concatenate_3 (Concatenate) global_max_pooling1d_1[0][0] global_max_pooling1d_2[0][0] global_max_pooling1d_3[0][0]	(None,	16424)	0	
global_max_poolingid_5[o][o]				flatten_1[0][0]
dense_3 (Dense) concatenate_3[0][0]	(None,	64)	1051200	
dropout_4 (Dropout)	(None,	64)	0	dense_3[0][0]
dense_4 (Dense)	(None,		195 =======	dropout_4[0][0]
Total params: 3,609,543 Trainable params: 1,579,743 Non-trainable params: 2,029,800				

```
[9]: validation_split_rate = 0.1
     skf = StratifiedKFold(n_splits=5,shuffle=True, random_state=42)
     Y = [np.argmax(y, axis=None, out=None) for y in Y_train]
     for tr_index, te_index in skf.split(X_train,Y):
         test_index = te_index
         train_index = tr_index
     trainRate = (len(train_index)/len(Y))*100
     testRate = (len(test index)/len(Y))*100
     print ("TrainRate:{:.2f}% testRate:{:.2f}% validation:{:.2f}% ".
      Gormat(trainRate,testRate, trainRate*validation_split_rate))
     X_train, X_test = X_train[train_index], X_train[test_index]
     pos_train1, pos_test1 = d1_train_embedded[train_index],__
      →d1_train_embedded[test_index]
    pos_train2, pos_test2 = d2_train_embedded[train_index],__
      →d2_train_embedded[test_index]
     y_train, y_test = Y_train[train_index], Y_train[test_index]
     # # Saving the training data split as a pickle file
     # training_data = {
           'X train': X train,
     #
           'pos_train1': pos_train1,
           'pos train2': pos train2,
           'y\_train': y\_train
     # }
     # with open('training_data12.pkl', 'wb') as f:
          pickle.dump(training_data, f)
     # # Saving the testing data split as a pickle file
     # testing_data = {
           'X test': X test,
           'pos_test1': pos_test1,
           'pos_test2': pos_test2,
           'y\_test': y\_test
     # }
     # with open('testing data12.pkl', 'wb') as f:
          pickle.dump(testing_data, f)
```

TrainRate:80.00% testRate:20.00% validation:8.00%

```
[10]: # Load the training data from the pickle file with open('training_data.pkl', 'rb') as f:
```

```
train_data = pickle.load(f)
# Load the testing data from the pickle file
with open('testing_data.pkl', 'rb') as f:
    test_data = pickle.load(f)
# Extract data from the loaded dictionaries
X_train = train_data['X_train']
pos_train1 = train_data['pos_train1']
pos_train2 = train_data['pos_train2']
y_train = train_data['y_train']
X_test = test_data['X_test']
pos_test1 = test_data['pos_test1']
pos_test2 = test_data['pos_test2']
y_test = test_data['y_test']
print(X_train.shape)
print(X_test.shape)
(4264, 81)
```

(4264, 81) (1066, 81)

4.0.7 Run the Evaluation using 10 fold Cross Validation

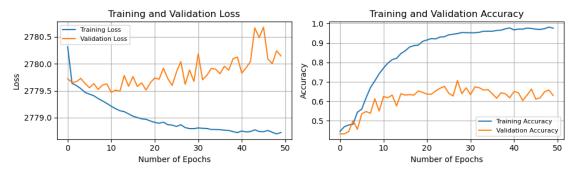
```
0.0709
Epoch 4/50
3837/3837 [=============== ] - 21s 5ms/step - loss: 2779.5398 -
acc: 0.4827 - f1: 0.2854 - val_loss: 2779.7274 - val_acc: 0.5012 - val_f1:
0.3381
Epoch 5/50
acc: 0.5442 - f1: 0.4584 - val_loss: 2779.6347 - val_acc: 0.4567 - val_f1:
0.4231
Epoch 6/50
3837/3837 [=============== ] - 21s 5ms/step - loss: 2779.4364 -
acc: 0.5603 - f1: 0.5021 - val_loss: 2779.5545 - val_acc: 0.5363 - val_f1:
0.5024
Epoch 7/50
acc: 0.6185 - f1: 0.5916 - val loss: 2779.6308 - val acc: 0.5480 - val f1:
0.5146
Epoch 8/50
acc: 0.6706 - f1: 0.6566 - val_loss: 2779.5228 - val_acc: 0.5386 - val_f1:
0.5019
Epoch 9/50
acc: 0.7047 - f1: 0.6950 - val_loss: 2779.6049 - val_acc: 0.6136 - val_f1:
0.5956
Epoch 10/50
acc: 0.7415 - f1: 0.7366 - val_loss: 2779.6261 - val_acc: 0.5504 - val_f1:
0.5353
Epoch 11/50
3837/3837 [============== ] - 23s 6ms/step - loss: 2779.2131 -
acc: 0.7709 - f1: 0.7635 - val_loss: 2779.4703 - val_acc: 0.6253 - val_f1:
0.6110
Epoch 12/50
acc: 0.7965 - f1: 0.7918 - val_loss: 2779.5100 - val_acc: 0.6183 - val_f1:
0.6134
Epoch 13/50
acc: 0.8144 - f1: 0.8134 - val_loss: 2779.4898 - val_acc: 0.6323 - val_f1:
0.6286
Epoch 14/50
acc: 0.8210 - f1: 0.8216 - val_loss: 2779.7811 - val_acc: 0.5761 - val_f1:
0.5672
Epoch 15/50
acc: 0.8455 - f1: 0.8457 - val_loss: 2779.5833 - val_acc: 0.6393 - val_f1:
```

```
0.6329
Epoch 16/50
acc: 0.8598 - f1: 0.8580 - val_loss: 2779.7611 - val_acc: 0.6323 - val_f1:
0.6300
Epoch 17/50
acc: 0.8791 - f1: 0.8780 - val_loss: 2779.5790 - val_acc: 0.6347 - val_f1:
0.6281
Epoch 18/50
acc: 0.8861 - f1: 0.8858 - val_loss: 2779.6440 - val_acc: 0.6323 - val_f1:
0.6332
Epoch 19/50
acc: 0.8887 - f1: 0.8867 - val_loss: 2779.5114 - val_acc: 0.6534 - val_f1:
0.6472
Epoch 20/50
acc: 0.9080 - f1: 0.9064 - val_loss: 2779.6474 - val_acc: 0.6464 - val_f1:
0.6400
Epoch 21/50
acc: 0.9150 - f1: 0.9139 - val_loss: 2779.7363 - val_acc: 0.6370 - val_f1:
0.6327
Epoch 22/50
acc: 0.9223 - f1: 0.9212 - val_loss: 2779.7114 - val_acc: 0.6370 - val_f1:
0.6398
Epoch 23/50
acc: 0.9208 - f1: 0.9202 - val_loss: 2779.9166 - val_acc: 0.6534 - val_f1:
0.6350
Epoch 24/50
acc: 0.9302 - f1: 0.9302 - val_loss: 2779.7252 - val_acc: 0.6674 - val_f1:
0.6565
Epoch 25/50
acc: 0.9317 - f1: 0.9309 - val_loss: 2779.5980 - val_acc: 0.6768 - val_f1:
0.6812
Epoch 26/50
3837/3837 [=============== ] - 21s 5ms/step - loss: 2778.8377 -
acc: 0.9416 - f1: 0.9413 - val loss: 2779.8469 - val acc: 0.6417 - val f1:
0.6401
Epoch 27/50
acc: 0.9445 - f1: 0.9445 - val loss: 2780.0383 - val acc: 0.6276 - val f1:
```

```
0.6256
Epoch 28/50
acc: 0.9481 - f1: 0.9484 - val_loss: 2779.6181 - val_acc: 0.7073 - val_f1:
0.7038
Epoch 29/50
acc: 0.9533 - f1: 0.9529 - val_loss: 2779.8841 - val_acc: 0.6393 - val_f1:
0.6300
Epoch 30/50
acc: 0.9526 - f1: 0.9523 - val_loss: 2779.6721 - val_acc: 0.6698 - val_f1:
0.6715
Epoch 31/50
acc: 0.9523 - f1: 0.9527 - val_loss: 2780.1814 - val_acc: 0.6347 - val_f1:
0.6350
Epoch 32/50
acc: 0.9520 - f1: 0.9520 - val_loss: 2779.7025 - val_acc: 0.6745 - val_f1:
0.6754
Epoch 33/50
acc: 0.9547 - f1: 0.9547 - val_loss: 2779.7859 - val_acc: 0.6698 - val_f1:
0.6690
Epoch 34/50
acc: 0.9599 - f1: 0.9592 - val_loss: 2779.9133 - val_acc: 0.6581 - val_f1:
0.6506
Epoch 35/50
acc: 0.9601 - f1: 0.9594 - val_loss: 2779.8988 - val_acc: 0.6604 - val_f1:
0.6692
Epoch 36/50
acc: 0.9599 - f1: 0.9603 - val_loss: 2779.8131 - val_acc: 0.6393 - val_f1:
0.6195
Epoch 37/50
acc: 0.9640 - f1: 0.9651 - val_loss: 2779.9524 - val_acc: 0.6159 - val_f1:
0.6145
Epoch 38/50
acc: 0.9653 - f1: 0.9668 - val loss: 2779.8813 - val acc: 0.6440 - val f1:
0.6390
Epoch 39/50
acc: 0.9724 - f1: 0.9723 - val loss: 2780.0892 - val acc: 0.6393 - val f1:
```

```
0.6354
Epoch 40/50
acc: 0.9768 - f1: 0.9771 - val_loss: 2780.1236 - val_acc: 0.6183 - val_f1:
0.6168
Epoch 41/50
acc: 0.9669 - f1: 0.9679 - val_loss: 2779.8234 - val_acc: 0.6511 - val_f1:
0.6406
Epoch 42/50
acc: 0.9711 - f1: 0.9718 - val loss: 2779.9257 - val acc: 0.6440 - val f1:
0.6478
Epoch 43/50
acc: 0.9708 - f1: 0.9711 - val loss: 2780.0395 - val acc: 0.6042 - val f1:
0.5988
Epoch 44/50
acc: 0.9760 - f1: 0.9762 - val_loss: 2780.6627 - val_acc: 0.6323 - val_f1:
0.6211
Epoch 45/50
acc: 0.9742 - f1: 0.9740 - val_loss: 2780.4818 - val_acc: 0.6628 - val_f1:
0.6643
Epoch 46/50
acc: 0.9705 - f1: 0.9707 - val_loss: 2780.6776 - val_acc: 0.6112 - val_f1:
0.6029
Epoch 47/50
acc: 0.9692 - f1: 0.9695 - val_loss: 2780.0895 - val_acc: 0.6183 - val_f1:
0.6127
Epoch 48/50
3837/3837 [============== ] - 21s 5ms/step - loss: 2778.7295 -
acc: 0.9729 - f1: 0.9744 - val_loss: 2780.0008 - val_acc: 0.6487 - val_f1:
0.6466
Epoch 49/50
acc: 0.9812 - f1: 0.9816 - val_loss: 2780.2382 - val_acc: 0.6581 - val_f1:
0.6499
Epoch 50/50
3837/3837 [============= ] - 20s 5ms/step - loss: 2778.7253 -
acc: 0.9755 - f1: 0.9758 - val loss: 2780.1437 - val acc: 0.6300 - val f1:
0.6374
```

```
[12]: import matplotlib.pyplot as plt
      # Training & Validation accuracy
      train_loss = history.history['loss']
      val_loss = history.history['val_loss']
      train_acc = history.history['acc']
      val_acc = history.history['val_acc']
      epochs = len(train_loss)
      xc = range(epochs)
      plt.figure(figsize=(10, 3))
      # Loss subplot
      plt.subplot(1, 2, 1)
      plt.plot(xc, train_loss, label='Training Loss')
      plt.plot(xc, val_loss, label='Validation Loss')
      plt.xlabel('Number of Epochs', fontsize=10)
      plt.ylabel('Loss', fontsize=10)
      plt.title('Training and Validation Loss', fontsize=12)
      plt.legend(fontsize=8)
      plt.grid(True)
      # Accuracy subplot
      plt.subplot(1, 2, 2)
      plt.plot(xc, train acc, label='Training Accuracy')
      plt.plot(xc, val_acc, label='Validation Accuracy')
      plt.xlabel('Number of Epochs', fontsize=10)
      plt.ylabel('Accuracy', fontsize=10)
      plt.title('Training and Validation Accuracy', fontsize=12)
      plt.legend(fontsize=8, loc='lower right') # Change position to lower right
      plt.grid(True)
      plt.tight_layout()
      plt.show()
```



```
[13]: import torch
      from sklearn.metrics import accuracy_score, classification_report,_
       →precision_recall_fscore_support
      # Predict on the training dataset
      train_predicted = np.argmax(model.predict([X_train, pos_train1, pos_train2]),__
       ⇒axis=1)
      y_train_to_label = np.argmax(y_train, axis=1)
      # Calculate accuracy, precision, recall, and F1-score for the training data
      train_accuracy = accuracy_score(y_train_to_label, train_predicted)
      train_prec, train_reca, train_fscore, _ = __
       ⇔precision_recall_fscore_support(y_train_to_label, train_predicted,_
       →average=param)
      # Print the classification report for the training data
      print("Training Classification Report:")
      print(classification_report(y_train_to_label, train_predicted))
      # Print the precision, recall, and F1-score for the training data
      print("Training Accuracy: {:.2f}%".format(train_accuracy * 100))
      print("Training Precision: {:.2f}%".format(train_prec * 100))
      print("Training Recall: {:.2f}%".format(train_reca * 100))
      print("Training F1 Score: {:.2f}%".format(train_fscore * 100))
```

Training Classification Report:

	precision	recall	f1-score	support
0	0.91 0.86	0.88 0.95	0.89 0.90	2023 1468
2	0.86	0.77	0.81	773
accuracy			0.88	4264
macro avg	0.88	0.86	0.87	4264
weighted avg	0.88	0.88	0.88	4264

Training Accuracy: 88.20% Training Precision: 87.62% Training Recall: 86.41% Training F1 Score: 86.85%

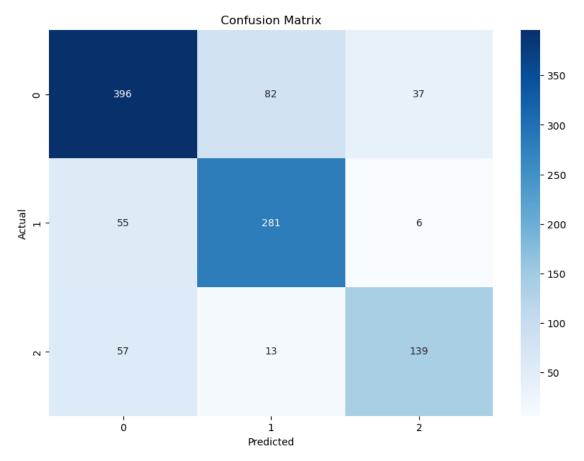
```
report_dict = classification_report(y_test_to_label, predicted,__
 ⇔output_dict=True)
# Create a new dictionary to hold the formatted values
formatted_report_dict = {}
# Iterate over the items in the report dictionary
for key, value in report dict.items():
    if isinstance(value, dict):
        # Format the nested dictionary values
        formatted_report_dict[key] = {sub_key: f"{sub_value:.4f}" for sub_key,__
 →sub_value in value.items()}
    else:
        # Format the top-level dictionary values
        formatted_report_dict[key] = f"{value:.4f}"
# Create a string representation of the formatted dictionary
formatted_report_str = classification_report(y_test_to_label, predicted,__
 ⇔digits=4)
# Print the formatted classification report
print(formatted_report_str)
print(" Precision:{:.2f}% Recall:{:.2f}% Fscore:{:.2f}% ".format(prec*100, ...

¬reca*100, fscore*100))
```

support	f1-score	recall	precision	
515	0.7742	0.7689	0.7795	0
342	0.7827	0.8216	0.7473	1
209	0.7110	0.6651	0.7637	2
1066	0.7655			accuracy
		0.7540	0 7005	accuracy
1066	0.7560	0.7519	0.7635	macro avg
1066	0.7645	0.7655	0.7661	weighted avg

Precision:76.35% Recall:75.19% Fscore:75.60%

```
[15]: import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.metrics import classification_report, confusion_matrix,
precision_recall_fscore_support
from sklearn.model_selection import StratifiedKFold
# Calculate and visualize the confusion matrix
cm = confusion_matrix(y_test_to_label, predicted)
plt.figure(figsize=(10, 7))
```



Precision:76.35% Recall:75.19% Fscore:75.60%

[]: