BeFree-2class EUADR LSTM

September 17, 2024

1 Evaluation using the BeFree corpus

1.0.1 EUADR dataset

The EU-ADR dataset contains annotations on drugs, diseases, genes and proteins, and associations between them. In this study, we used only GDAs to evaluate the method. Each association is classified according to its level of certainty as positive association (PA), negative association (NA), speculative association (SA); or false association (FA). The EU-ADR corpus is based on 100 MEDLINE abstracts for each association set, and its annotation was conducted by three experts.

2 ————

3 imports

```
[1]: import tensorflow as tf
     from keras.models import load_model
     from keras.callbacks import ModelCheckpoint, EarlyStopping
     from keras_tqdm import TQDMNotebookCallback
     import numpy as np
     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
     from keras.layers.convolutional import Conv2D, MaxPooling2D
     from tensorflow.keras.utils import to_categorical
     from 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 *
```

Using TensorFlow backend.

3.0.1 Define Callback functions to generate Mesures

```
[2]: 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 8

4.0.1 Load Prerocssed Data

```
d2_train = pickle.load(handle)
print("d2_train",len(d2_train))
Y_train = pickle.load(handle)
print("Y_train",len(d2_train))
Tr_word_list = pickle.load(handle)
print("Tr_word_list",len(d2_train))
word_vectors = pickle.load(handle)
print("word_vectors",len(word_vectors))
word_dict = pickle.load(handle)
print("word_dict",len(word_dict))
d1 dict = pickle.load(handle)
print("d1_dict",len(d1_dict))
d2_dict = pickle.load(handle)
print("d2_dict",len(d2_dict))
label_dict = pickle.load(handle)
print("label_dict",len(label_dict))
MAX_SEQUENCE_LENGTH = pickle.load(handle)
print("MAX_SEQUENCE_LENGTH", MAX_SEQUENCE_LENGTH)
```

```
W_train 355
d1_train 355
d2_train 355
Y_train 355
Tr_word_list 355
word_vectors 1355
word_dict 1355
d1_dict 169
d2_dict 171
label_dict 4
MAX_SEQUENCE_LENGTH 102
```

4.0.2 Create Position Embedding Vectors

```
[4]: import keras
from keras_pos_embd import TrigPosEmbedding

model = keras.models.Sequential()
model.add(TrigPosEmbedding(
    input_shape=(None,),
    output_dim=20,  # The dimension of embeddings.
    mode=TrigPosEmbedding.MODE_EXPAND, # Use `expand` mode
    name='Pos-Embd',
))
model.compile('adam', keras.losses.mae, {})
model.summary()

d1_train_embedded=model.predict(d1_train)
```

4.0.3 Prepare Word Embedding Layer

4.0.4 Prepare Attention Mechanism

```
[6]: INPUT_DIM = 2
    TIME_STEPS = MAX_SEQUENCE_LENGTH

[7]: def attentionNew(inputs):
    inputs = Lambda(lambda x: tf.keras.backend.sigmoid(x))(inputs)
    input_dim = int(inputs.shape[2])
    a = Permute((2, 1))(inputs)
    a = Dense(TIME_STEPS, activation='softmax')(a)
    a_probs = Permute((2, 1))(a)
    output_attention_mul = multiply([inputs, a_probs])
    output_attention_mul = Lambda(lambda x: tf.keras.backend.
    sigmoid(x))(output_attention_mul)
    return output_attention_mul
```

4.0.5 Create the Model

```
[8]: dropRate=0.1
     param='binary'
     def build_model_positionAttention():
         sequence_input = Input(shape=(MAX_SEQUENCE_LENGTH,), dtype='int32')
      embedding_layer=create_embedding_layer(use_pretrained=True,is_trainable=False)
         embedded sequences = embedding layer(sequence input)
        pos_embedd_1=Input(shape=(MAX_SEQUENCE_LENGTH,20), dtype='float32')
        pos_embedd_2=Input(shape=(MAX_SEQUENCE_LENGTH,20), dtype='float32')
        embedded_sequences =
      ⇒concatenate([embedded_sequences,pos_embedd_1,pos_embedd_2])
        x = Conv1D(128, 7, activation='relu')(embedded_sequences)
        x = MaxPooling1D(3)(x)
        x = Dropout(0.5)(x)
        x = Conv1D(64, 5, activation='relu')(x)
        x = MaxPooling1D(3)(x)
        x = Dropout(0.5)(x)
        conv_sequence_7=GlobalMaxPooling1D()(x) #x = Flatten()(x)
        forward = LSTM(100, recurrent_dropout=0.05)(embedded_sequences)
```

```
backward = LSTM(100, go_backwards=True,recurrent_dropout=0.
    ⇔05) (embedded_sequences)
      lstm_sequence = concatenate([forward,backward])
      merge = concatenate([conv_sequence_7,lstm_sequence])
      x = Dropout(dropRate)(x)
      x = Dense(256, activation='relu', kernel_regularizer=regularizers.12(0.
    →05))(merge)
      x = Dropout(0.1)(x)
      preds = Dense(2, activation='softmax')(x)
      model = Model(inputs=[sequence_input,__
    →pos_embedd_1,pos_embedd_2],outputs=preds)
    acompile(loss='binary_crossentropy',optimizer='adam',metrics=['acc',f1])
      #model.summary()
      return model
[9]: model = build_model_positionAttention()
   model.summary()
   Model: "model 1"
   Layer (type)
                          Output Shape Param # Connected to
   ______
   _____
   input 1 (InputLayer)
                       (None, 102) 0
   ______
   embedding_1 (Embedding)
                      (None, 102, 200) 271000 input_1[0][0]
   input_2 (InputLayer)
                          (None, 102, 20)
   input_3 (InputLayer)
                           (None, 102, 20)
   ______
   concatenate_1 (Concatenate) (None, 102, 240) 0
   embedding_1[0][0]
                                                     input_2[0][0]
                                                     input_3[0][0]
```

conv1d_1 (Conv1D) concatenate_1[0][0]		96, 128)		
max_pooling1d_1 (MaxPooling1D)				conv1d_1[0][0]
dropout_1 (Dropout) max_pooling1d_1[0][0]		32, 128)		
conv1d_2 (Conv1D)	(None,	28, 64)	41024	dropout_1[0][0]
max_pooling1d_2 (MaxPooling1D)			0	conv1d_2[0][0]
dropout_2 (Dropout) max_pooling1d_2[0][0]	(None,	9, 64)	0	
lstm_1 (LSTM) concatenate_1[0][0]	(None,	100)	136400	
lstm_2 (LSTM) concatenate_1[0][0]	(None,	100)	136400	
global_max_pooling1d_1 (GlobalM	(None,	64)	0	dropout_2[0][0]
concatenate_2 (Concatenate)			0	lstm_1[0][0] lstm_2[0][0]
concatenate_3 (Concatenate) global_max_pooling1d_1[0][0] concatenate_2[0][0]	(None,	264)	0	
dense_1 (Dense) concatenate_3[0][0]	(None,		67840	
dropout_4 (Dropout)	(None,		0	dense_1[0][0]

4.0.6 Run the Evaluation using 10 fold Cross Validation

```
[10]: validation_split_rate=0.1
      skf = StratifiedKFold(n_splits=5, random_state=None)
      Y = [np.argmax(y, axis=None, out=None) for y in Y_train]
      #print(len(Y))
      all histories=[]
      for trI, teI in skf.split(W_train,Y):
          train_index =trI
          test_index =teI
      trainRate = (len(train_index)/len(Y))*100
      testRate = (len(test_index)/len(Y))*100
      print ("TrainRate:{:.2f}% testRate:{:.2f}% validation:{:.2f}% ".

¬format(trainRate,testRate, trainRate*validation_split_rate))

      #print(train index, test index)
      X_train, X_test = W_train[train_index], W_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_data.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_data.pkl', 'wb') as f:
# pickle.dump(testing_data, f)
```

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

```
[11]: # 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)
```

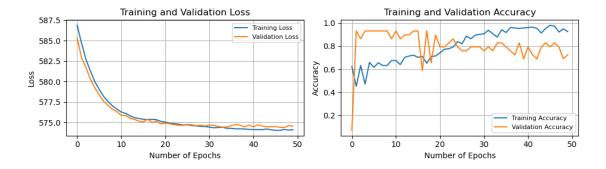
(284, 102)

```
Epoch 2/50
0.4510 - f1: 0.4512 - val_loss: 582.9426 - val_acc: 0.9310 - val_f1: 0.9310
Epoch 3/50
acc: 0.6314 - f1: 0.6307 - val_loss: 581.7048 - val_acc: 0.8621 - val_f1: 0.8621
acc: 0.4706 - f1: 0.4714 - val_loss: 580.2935 - val_acc: 0.9310 - val_f1: 0.9310
Epoch 5/50
acc: 0.6588 - f1: 0.6589 - val_loss: 579.2651 - val_acc: 0.9310 - val_f1: 0.9310
Epoch 6/50
acc: 0.6157 - f1: 0.6154 - val_loss: 578.3752 - val_acc: 0.9310 - val_f1: 0.9310
Epoch 7/50
0.6549 - f1: 0.6547 - val_loss: 577.6010 - val_acc: 0.9310 - val_f1: 0.9310
Epoch 8/50
255/255 [============= ] - 5s 21ms/step - loss: 577.5770 - acc:
0.6314 - f1: 0.6307 - val_loss: 577.0852 - val_acc: 0.9310 - val_f1: 0.9310
Epoch 9/50
0.6314 - f1: 0.6313 - val_loss: 576.6284 - val_acc: 0.9310 - val_f1: 0.9310
Epoch 10/50
0.6745 - f1: 0.6738 - val_loss: 576.3329 - val_acc: 0.8621 - val_f1: 0.8621
Epoch 11/50
0.6745 - f1: 0.6741 - val_loss: 575.8536 - val_acc: 0.9310 - val_f1: 0.9310
Epoch 12/50
0.6392 - f1: 0.6394 - val_loss: 575.8679 - val_acc: 0.8621 - val_f1: 0.8621
Epoch 13/50
0.7020 - f1: 0.7016 - val_loss: 575.5275 - val_acc: 0.8966 - val_f1: 0.8966
Epoch 14/50
0.7137 - f1: 0.7140 - val_loss: 575.3867 - val_acc: 0.8966 - val_f1: 0.8966
Epoch 15/50
0.7216 - f1: 0.7216 - val_loss: 575.1622 - val_acc: 0.9310 - val_f1: 0.9310
0.7020 - f1: 0.7031 - val_loss: 575.0663 - val_acc: 0.9310 - val_f1: 0.9310
Epoch 17/50
0.7098 - f1: 0.7089 - val_loss: 575.3945 - val_acc: 0.5862 - val_f1: 0.5862
```

```
Epoch 18/50
0.6510 - f1: 0.6512 - val_loss: 574.9982 - val_acc: 0.9310 - val_f1: 0.9310
Epoch 19/50
0.7098 - f1: 0.7092 - val_loss: 575.1613 - val_acc: 0.6552 - val_f1: 0.6552
Epoch 20/50
0.7137 - f1: 0.7136 - val_loss: 574.8128 - val_acc: 0.8966 - val_f1: 0.8966
Epoch 21/50
0.7412 - f1: 0.7409 - val_loss: 574.9236 - val_acc: 0.7931 - val_f1: 0.7931
Epoch 22/50
0.7725 - f1: 0.7729 - val_loss: 574.8499 - val_acc: 0.7931 - val_f1: 0.7931
Epoch 23/50
0.7765 - f1: 0.7768 - val_loss: 574.7311 - val_acc: 0.8276 - val_f1: 0.8276
Epoch 24/50
0.7922 - f1: 0.7923 - val_loss: 574.6774 - val_acc: 0.8621 - val_f1: 0.8621
Epoch 25/50
0.8392 - f1: 0.8388 - val_loss: 574.6389 - val_acc: 0.7931 - val_f1: 0.7931
Epoch 26/50
0.8196 - f1: 0.8202 - val_loss: 574.7734 - val_acc: 0.7586 - val_f1: 0.7586
Epoch 27/50
0.8863 - f1: 0.8863 - val_loss: 574.7174 - val_acc: 0.7586 - val_f1: 0.7586
Epoch 28/50
0.8627 - f1: 0.8630 - val_loss: 574.6096 - val_acc: 0.7931 - val_f1: 0.7931
Epoch 29/50
0.8941 - f1: 0.8942 - val_loss: 574.6714 - val_acc: 0.7931 - val_f1: 0.7931
Epoch 30/50
0.9020 - f1: 0.9017 - val_loss: 574.5762 - val_acc: 0.7931 - val_f1: 0.7931
Epoch 31/50
0.9059 - f1: 0.9052 - val_loss: 574.6773 - val_acc: 0.7586 - val_f1: 0.7586
0.9373 - f1: 0.9372 - val_loss: 574.6636 - val_acc: 0.7931 - val_f1: 0.7931
Epoch 33/50
0.9059 - f1: 0.9059 - val_loss: 574.5253 - val_acc: 0.7586 - val_f1: 0.7586
```

```
Epoch 34/50
0.8784 - f1: 0.8785 - val_loss: 574.4338 - val_acc: 0.8276 - val_f1: 0.8276
Epoch 35/50
0.9412 - f1: 0.9412 - val_loss: 574.4556 - val_acc: 0.8276 - val_f1: 0.8276
Epoch 36/50
0.9176 - f1: 0.9177 - val_loss: 574.6126 - val_acc: 0.7931 - val_f1: 0.7931
Epoch 37/50
0.9608 - f1: 0.9609 - val_loss: 574.7714 - val_acc: 0.7586 - val_f1: 0.7586
Epoch 38/50
0.9569 - f1: 0.9570 - val_loss: 574.6733 - val_acc: 0.7241 - val_f1: 0.7241
Epoch 39/50
acc: 0.9529 - f1: 0.9529 - val_loss: 574.4665 - val_acc: 0.8276 - val_f1: 0.8276
Epoch 40/50
acc: 0.9569 - f1: 0.9568 - val_loss: 574.6920 - val_acc: 0.6897 - val_f1: 0.6897
Epoch 41/50
acc: 0.9608 - f1: 0.9603 - val_loss: 574.4649 - val_acc: 0.7931 - val_f1: 0.7931
Epoch 42/50
acc: 0.9647 - f1: 0.9648 - val_loss: 574.7181 - val_acc: 0.7241 - val_f1: 0.7241
Epoch 43/50
255/255 [============= ] - 132s 519ms/step - loss: 574.1348 -
acc: 0.9529 - f1: 0.9530 - val_loss: 574.5671 - val_acc: 0.6897 - val_f1: 0.6897
Epoch 44/50
0.9137 - f1: 0.9141 - val_loss: 574.4708 - val_acc: 0.7931 - val_f1: 0.7931
Epoch 45/50
0.9529 - f1: 0.9530 - val_loss: 574.5026 - val_acc: 0.8276 - val_f1: 0.8276
Epoch 46/50
0.9804 - f1: 0.9805 - val_loss: 574.4952 - val_acc: 0.7931 - val_f1: 0.7931
Epoch 47/50
0.9725 - f1: 0.9727 - val_loss: 574.4174 - val_acc: 0.8276 - val_f1: 0.8276
0.9216 - f1: 0.9219 - val_loss: 574.3728 - val_acc: 0.7931 - val_f1: 0.7931
Epoch 49/50
```

```
0.9490 - f1: 0.9488 - val_loss: 574.6471 - val_acc: 0.6897 - val_f1: 0.6897
     Epoch 50/50
     0.9255 - f1: 0.9255 - val_loss: 574.5488 - val_acc: 0.7241 - val_f1: 0.7241
[]:
[13]: 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()
```



```
[14]: 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, _ = __
       oprecision_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	0.96	0.93	89
1	0.98	0.96	0.97	195
accuracy			0.96	284
macro avg	0.95	0.96	0.95	284
weighted avg	0.96	0.96	0.96	284

Training Accuracy: 95.77%

```
Training Precision: 97.91%
Training Recall: 95.90%
Training F1 Score: 96.89%
```

```
[]:
 []:
[17]: | predicted = np.argmax(model.predict([X_test,pos_test1,pos_test2]), axis=1)
      y_test_to_label= np.argmax(y_test, axis=1)
      prec, reca, fscore, sup = precision_recall_fscore_support(y_test_to_label,__
       ⇒predicted, average=param)
      # Generate the classification report as a dictionary
      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,_u

digits=4)

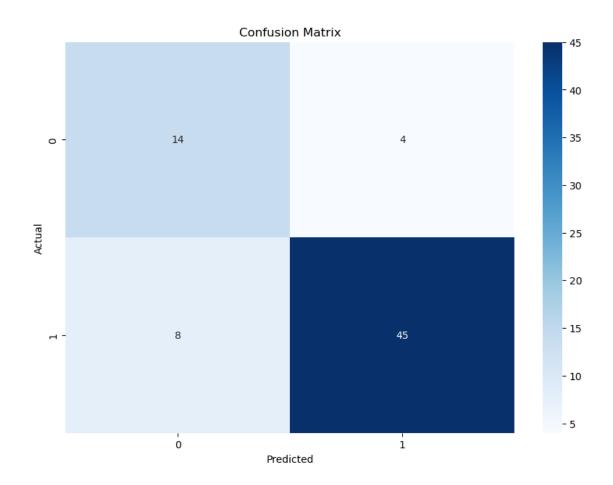
      # Print the formatted classification report
      print(formatted_report_str)
      print(" Precision:{:.2f}% Recall:{:.2f}% Fscore:{:.2f}% ".format(prec*100, __
       ⇔reca*100, fscore*100))
```

support	f1-score	recall	precision	
18	0.6829	0.7778	0.6087	0
53	0.8713	0.8302	0.9167	1
71	0.8169			accuracy

```
macro avg 0.7627 0.8040 0.7771 71 weighted avg 0.8386 0.8169 0.8235 71
```

Precision:91.67% Recall:83.02% Fscore:87.13%

```
[16]: 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))
      sns.heatmap(cm, annot=True, fmt='d', cmap='Blues', xticklabels=['0', '1'],
       ⇔yticklabels=['0', '1'])
      plt.xlabel('Predicted')
      plt.ylabel('Actual')
      plt.title('Confusion Matrix')
      plt.show()
      # Print precision, recall, and f-score
      prec, reca, fscore, sup = precision_recall_fscore_support(y_test_to_label,__
       →predicted, average=param)
      print(" Precision:{:.2f}% Recall:{:.2f}% Fscore:{:.2f}% ".format(prec*100,__
       →reca*100, fscore*100))
```



Precision:91.84% Recall:84.91% Fscore:88.24%

[]: