Pfam_seed_random_split_new_2

July 7, 2019

1 Protein Family Classification

1.1 1.1 Description

The directory contains data to train a model to predict the function of protein domains, based on the PFam dataset.

Domains are functional sub-parts of proteins; much like images in ImageNet are pre segmented to contain exactly one object class, this data is presegmented to contain exactly and only one domain.

The purpose of the dataset is to repose the PFam seed dataset as a multiclass classification machine learning task.

The task is: given the amino acid sequence of the protein domain, predict which class it belongs to. There are about 1 million training examples, and 18,000 output classes.

1.2 Problem Statement:

Given the amino acid sequence of the protein domain, predict which class it belongs to.

1.2 Sources https://www.kaggle.com/googleai/pfam-seed-random-split

1.3 2. Data Overview

The approach used to partition the data into training/dev/testing folds is a random split.

- Training data should be used to train your models.
- Dev (development) data should be used in a close validation loop (maybe for hyperparameter tuning or model validation).
- Test data should be reserved for much less frequent evaluations - this helps avoid overfitting on your test data, as it should only be used infrequently.

Each fold (train, dev, test) has a number of files in it. Each of those files contains csv on each line, which has the following fields:

- sequence: HWLQMRDSMNTYNNMVNRCFATCIRSFQEKKVNAEEMDCTKRCVTKFV-GYSQRVALRFAE

- family_accession: PF02953.15

- sequence_name: C5K6N5_PERM5/28-87

- aligned_sequence: ....HWLQMRDSMNTYNNMVNRCFATCI...........RS.F....QEKKVNAEE.....MDCT....KRCV
- family_id: zf-Tim10_DDP

Description of fields: -

- sequence: These are usually the input features to your model. Amino acid sequence for this domain. There are 20 very common amino acids (frequency > 1,000,000), and 4 amino acids that are quite uncommon: X, U, B, O, Z.
- family_accession: These are usually the labels for your model. Accession number in form PFxxxxx.y (Pfam), where xxxxx is the family accession, and y is the version number. Some values of y are greater than ten, and so 'y' has two digits.
- family_id: One word name for family
- sequence_name: Sequence name, in the form "$uniprot_accession_id/$start_index-$end_index".
- aligned_sequence: Contains a single sequence from the multiple sequence alignment (with the rest of the members of the family in seed, with gaps retained.
- Generally, the family_accession field is the label, and the sequence (or aligned sequence) is the training feature.

1.3.1 2.2.2 Performance Metric

Metric(s): Micro F1 score, Accuracy
source : Mean F Score

1.4 Exploratory Data Analysis

```
In [10]: import tensorflow as tf
         tf.logging.set_verbosity(tf.logging.WARN)
         import matplotlib.pyplot as plt # plotting
         import numpy as np # linear algebra
         import os # accessing directory structure
         import pandas as pd # data processing, CSV file I/O (e.g. pd.read_csv)
         import seaborn
         from Bio.SeqUtils import seq3
         from keras.layers.normalization import BatchNormalization
         from keras.layers import Dropout
         from sklearn.feature_extraction.text import CountVectorizer
         from sklearn.feature_extraction.text import TfidfVectorizer
         from tqdm import tqdm
         from sklearn.preprocessing import LabelEncoder
         from sklearn.preprocessing import OneHotEncoder
         from keras.utils import np_utils
         from keras.datasets import mnist
         import seaborn as sns
         from keras.initializers import RandomNormal
```

```
        from keras.models import Sequential
        from keras.layers import Activation,Dense
        import matplotlib.pyplot as plt
        from keras.callbacks import EarlyStopping
        from keras.callbacks import ModelCheckpoint
        from keras.models import load_model
        from keras.layers import LSTM
        from keras.layers.embeddings import Embedding
        from sklearn.metrics import f1_score
        from keras.preprocessing import sequence
        max_review_length = 100
        import warnings
        from tqdm import tqdm
        warnings.filterwarnings('ignore')
```

1.5 Loading the data

```
In [11]: data_partitions_dirpath = 'random_split/'
         print('Available dataset partitions: ', os.listdir(data_partitions_dirpath))
```

```
Available dataset partitions:  ['dev', 'test', 'train']
```

```
In [12]: #reading the files
         def read_all_shards(partition='dev', data_dir=data_partitions_dirpath):
             shards = []
             for fn in os.listdir(os.path.join(data_dir, partition)):
                 with open(os.path.join(data_dir, partition, fn)) as f:
                     shards.append(pd.read_csv(f, index_col=None))
             return pd.concat(shards)

         test = read_all_shards('test')
         dev = read_all_shards('dev')
         train = read_all_shards('train')

         partitions = {'test': test, 'dev': dev, 'train': train}
         for name, df in partitions.items():
             print('Dataset partition "%s" has %d sequences' % (name, len(df)))
```

```
Dataset partition "test" has 126171 sequences
Dataset partition "dev" has 126171 sequences
Dataset partition "train" has 1086741 sequences
```

```
In [4]: train.head()
```

```
Out[4]:     family_id         sequence_name family_accession  \
        0  Gly_kinase    Q07ZT2_SHEFN/3-383       PF02595.15
        1   Pkinase_C  F2UES8_SALR5/486-527       PF00433.24
```

```
2     DUF3384   J9LUZ1_ACYPI/51-475        PF11864.8
3      FKBP_N   F5YQG8_TREPZ/38-136       PF01346.18
4         PAZ   PIWL2_XENTR/368-498       PF02170.22

                                       aligned_sequence  \
0  IVIAPDSFKESLSALEVANAIEDGFKQ...
1  LKDPLDTSNF..DE...DFTSLPAVDTPVE...
2  IHTRIKAIKELAE.VAKSHR...LEENAVASLWLRVHD.LFSH...
3  DKDVGYAIGM...FIG...SE...
4  LDIMNILYQ...Q..SPEN...FQ...

                                               sequence
0  IVIAPDSFKESLSALEVANAIEDGFKQVFPNAQYCKVPMADGGEGT...
1         LKDPLDTSNFDEDFTSLPAVDTPVEDSGLSQSVQRKFEGFSF
2  IHTRIKAIKELAEVAKSHRLEENAVASLWLRVHDLFSHHVPKEDRH...
3  DKDVGYAIGMFIGSEYKQQGQLSMITVDYDAFTRGFKDALEGNETA...
4  LDIMNILYQQSPENFQDEVTKQLVGSIVITRYNNRTYRIDDIEWNM...
```

```
In [0]: print('There are {} output classes in train data'.format(train.family_accession.drop_du
        print('There are {} output classes in dev data'.format(dev.family_accession.drop_dupli
```

```
There are 17929 output classes in train data
There are 13071 output classes in dev data
```

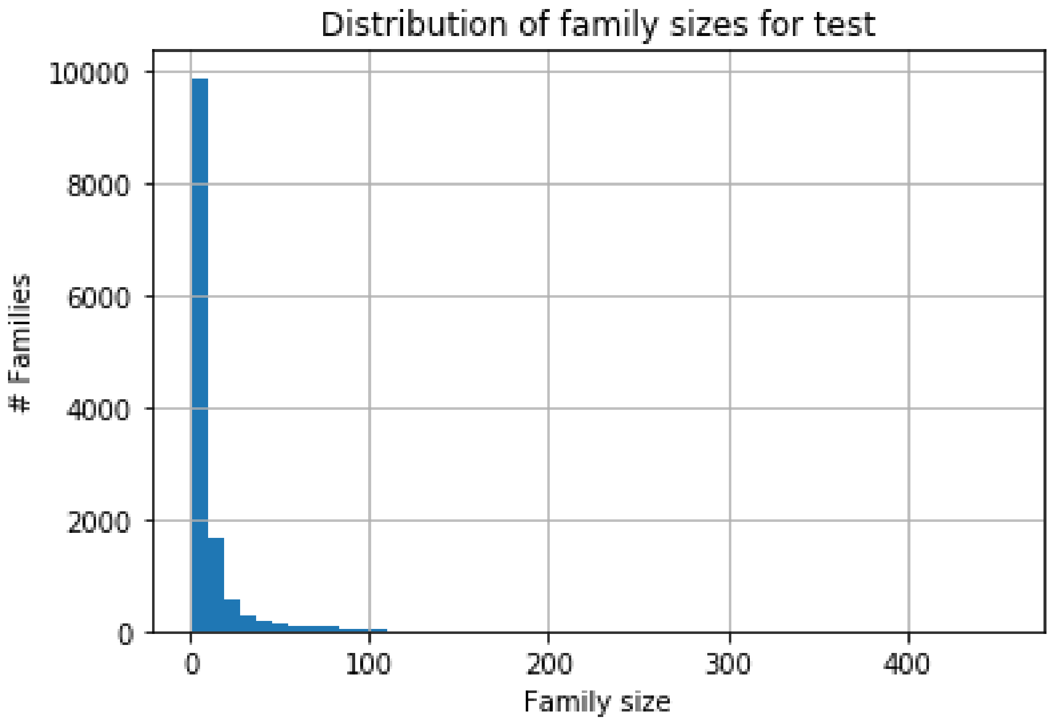
1.5.1 Families with the most sequences

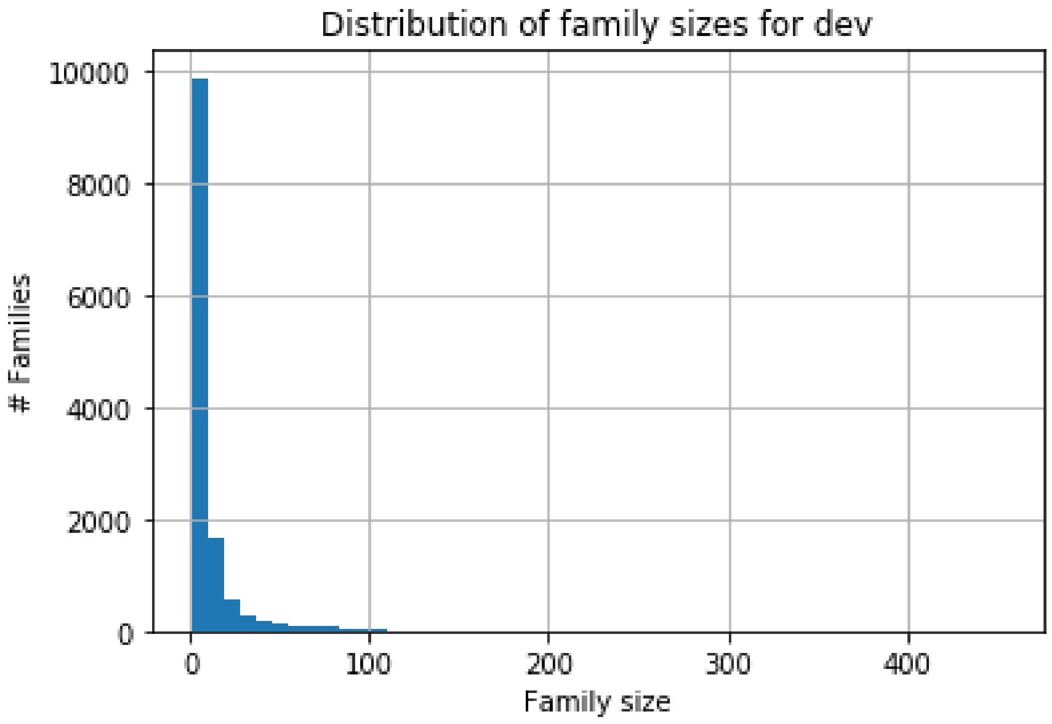
```
In [4]: train.groupby('family_id').size().sort_values(ascending=False).head(10)
```

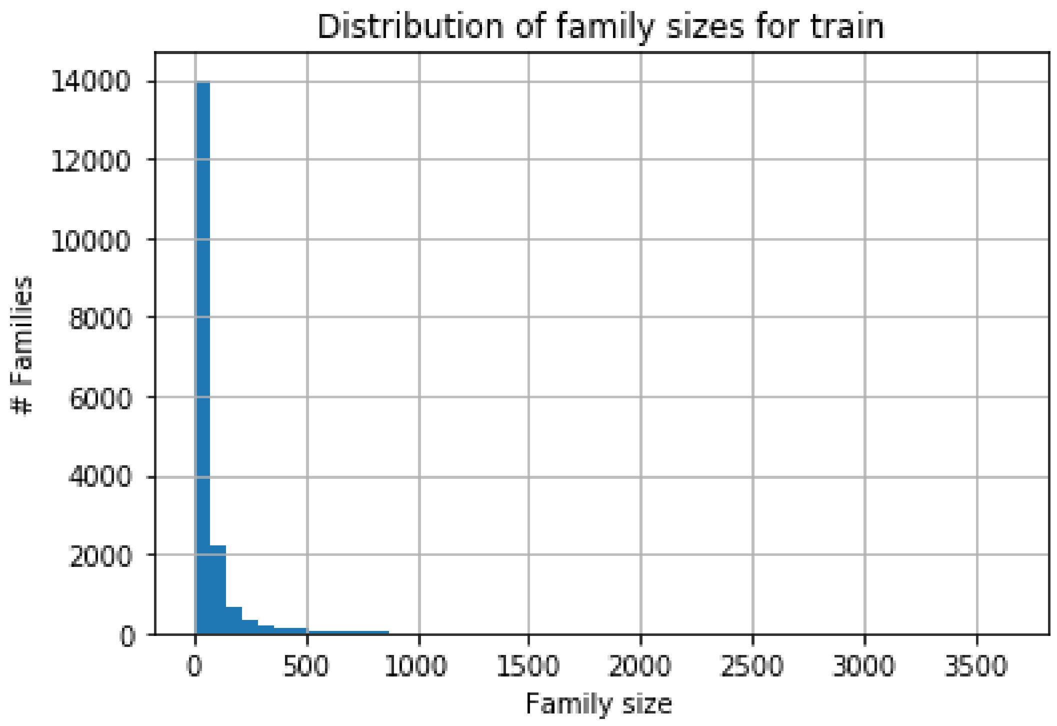
```
Out[4]: family_id
        Methyltransf_25    3637
        LRR_1              1927
        Acetyltransf_7     1761
        His_kinase         1537
        Bac_transf         1528
        Lum_binding        1504
        DNA_binding_1      1345
        Chromate_transp    1265
        Lipase_GDSL_2      1252
        DnaJ_CXXCXGXG      1210
        dtype: int64
```

We can see that Methyltransf_25 is the most common family

```
In [0]: for name, partition in partitions.items():
            partition.groupby('family_id').size().hist(bins=50)
            plt.title('Distribution of family sizes for %s' % name)
            plt.ylabel('# Families')
            plt.xlabel('Family size')
            plt.show()
```


Distribution of family sizes for test
10000
8000
6000
4000
2000
0
# Families
0
100
200
300
400
Family size

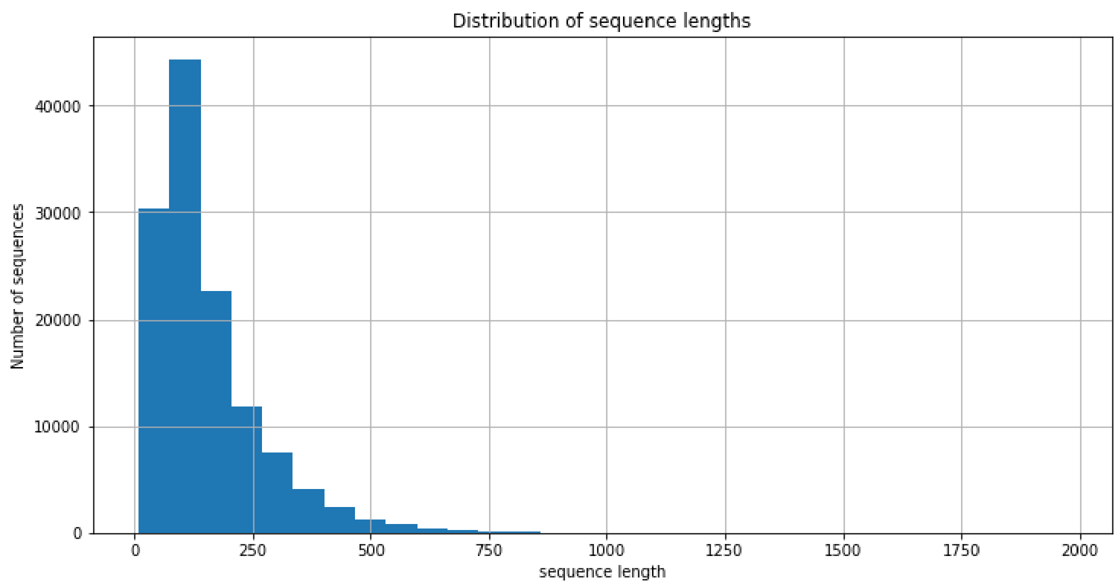

Distribution of family sizes for dev
10000
8000
6000
4000
2000
0
# Families
0
100
200
300
400
Family size



We can see that the train test and dev have same distribution.

1.5.2 Families with the longest sequence length

```
In [0]: fig = plt.subplots(figsize=(12, 6))
        dev['sequence'] = dev.sequence.str.len()
        dev.sequence.hist(bins=30)
        plt.title('Distribution of sequence lengths')
        plt.xlabel('sequence length')
        plt.ylabel('Number of sequences')

Out[0]: Text(0, 0.5, 'Number of sequences')
```



We can see that the average length of sequence is around 200

```
In [0]: family_lengths = (dev[['family_id', 'sequence']]
                           .drop_duplicates()
                           .sort_values(by='sequence', ascending=False))

        family_lengths.head(5)

Out[0]:       family_id  sequence
        9434      GREB1      1971
        6702     Nup192      1910
        11512    Nup192      1855
        7972     Nup192      1750
        3109     Nup192      1676
```

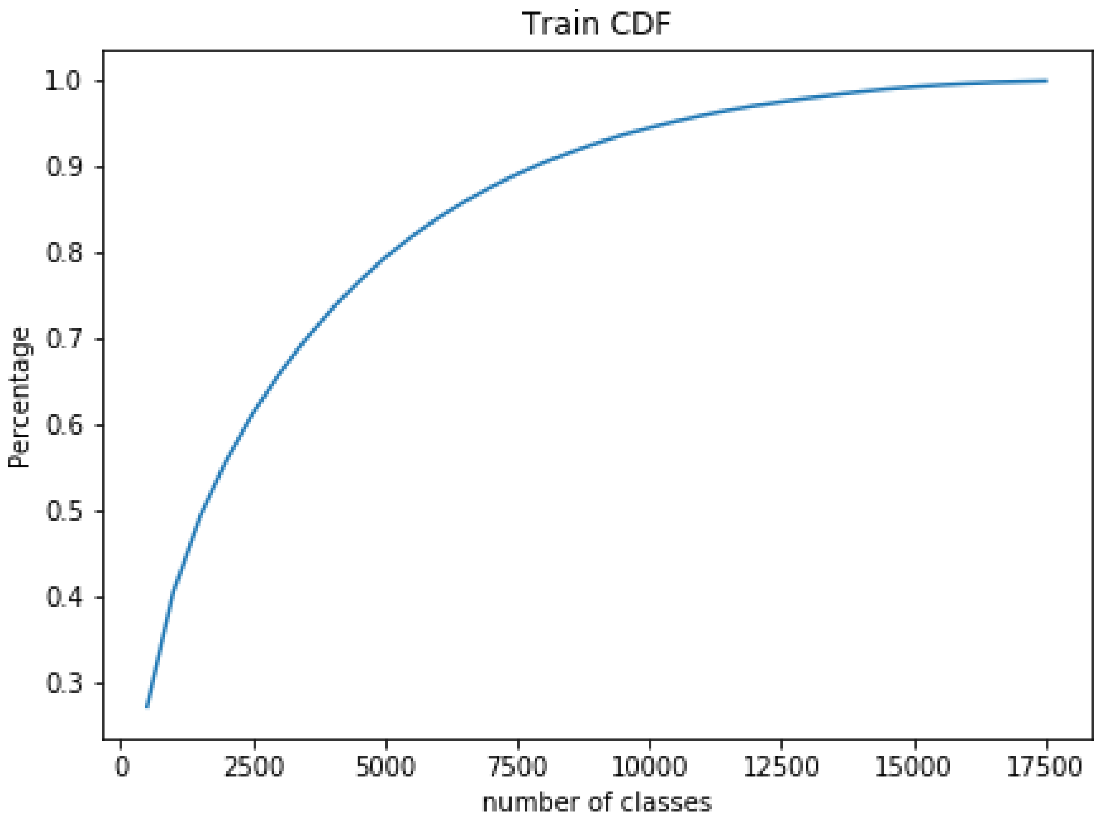
The family GREB1 has the longest sequence of length 1971

```
In [0]: family_lengths = (dev[['family_id', 'sequence']]
                           .drop_duplicates()
                           .sort_values(by='sequence', ascending=True))

        family_lengths.head(5)

Out[0]:           family_id  sequence
        5508            YLP         9
        9947           LSPR         9
        6021     Involucrin         9
        6137  Sperm_act_pep        10
        6137           FARP        10
```

The family GREB1 has the longest sequence of length 1971

1.5.3 CDF of family accessions

```
In [0]: fig = plt.subplots(figsize=(7, 5))
        train_range={}
        for i in range(500,18000,500):
            train_top=train.groupby('family_id').size().sort_values(ascending=False).head(i)
            train_range[i]=train_top.values.sum()/1086741
        plt.plot(train_range.keys(),train_range.values())
        plt.xlabel('number of classes')
        plt.ylabel('Percentage')
        plt.title('Train CDF')
        plt.show()
```

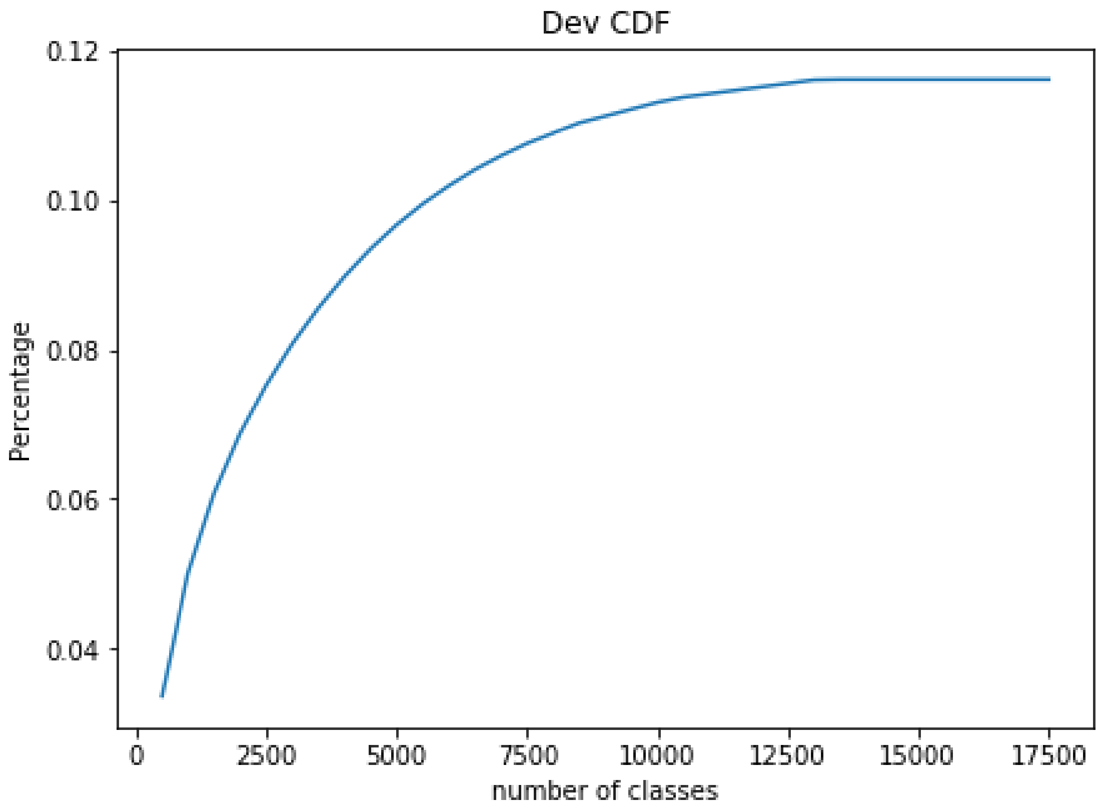


We consider only 1000 classes as it covers almost 40% of the data and also to reduce computation time

```
In [13]: train_top=train.groupby('family_id').size().sort_values(ascending=False).head(1000)
         print('1000 classes cover {}% of train data'.format(train_top.values.sum()/train.shap
```

```
1000 classes cover 40.44137471577864% of train data
```

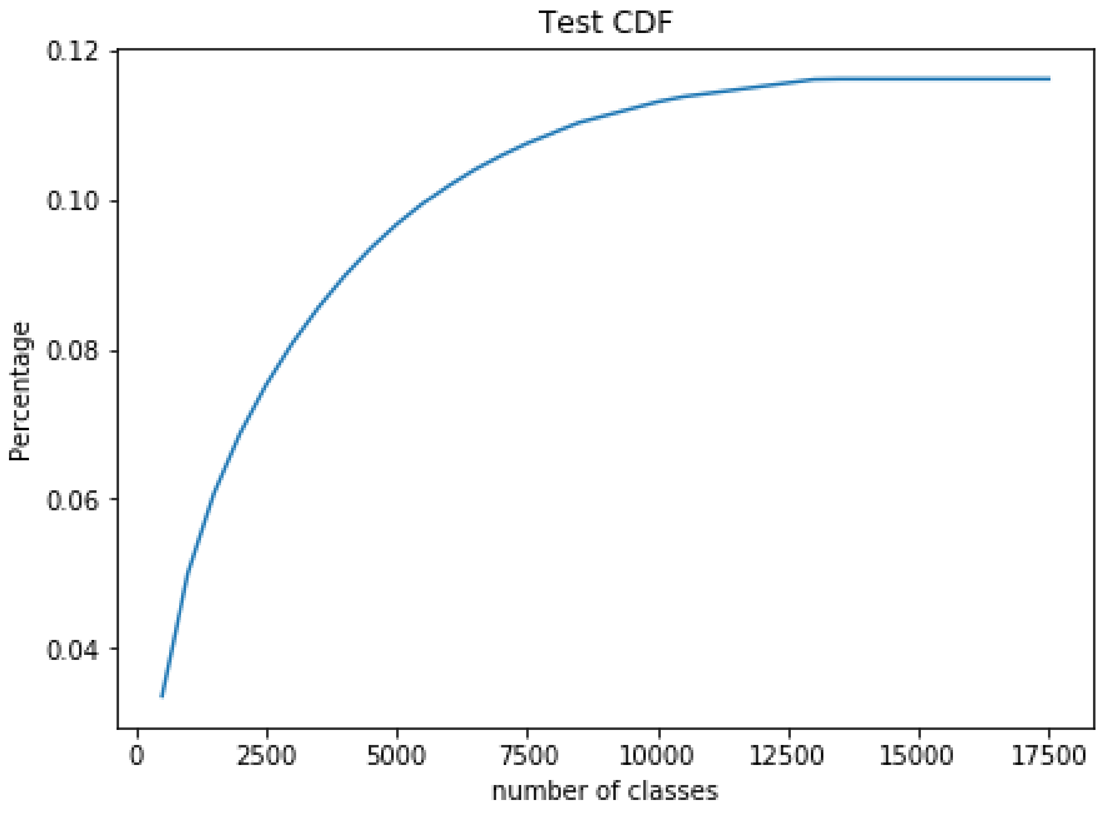
```
In [0]: fig = plt.subplots(figsize=(7, 5))
        dev_range={}
        for i in range(500,18000,500):
            dev_top=dev.groupby('family_id').size().sort_values(ascending=False).head(i)
            dev_range[i]=dev_top.values.sum()/1086741
        plt.plot(dev_range.keys(),dev_range.values())
        plt.xlabel('number of classes')
        plt.ylabel('Percentage')
        plt.title('Dev CDF')
        plt.show()
```



```
In [14]: dev_top=dev.groupby('family_id').size().sort_values(ascending=False).head(800)

          print('800 classes cover {}% of dev data'.format(dev_top.values.sum()/dev.shape[0]*10
```

```
800 classes cover 38.251262175935835% of dev data
```

```
In [0]: fig = plt.subplots(figsize=(7, 5))
        test_range={}
        for i in range(500,18000,500):
            test_top=dev.groupby('family_id').size().sort_values(ascending=False).head(i)
            test_range[i]=test_top.values.sum()/1086741
        plt.plot(test_range.keys(),test_range.values())
        plt.xlabel('number of classes')
        plt.ylabel('Percentage')
        plt.title('Test CDF')
        plt.show()
```



We consider only 4500 classes as it covers 80% of the dev and test data

```
In [15]: test_top=test.groupby('family_id').size().sort_values(ascending=False).head(800)

         print('800 classes cover {}% of test data'.format(test_top.values.sum()/test.shape[0]
```

```
800 classes cover 38.251262175935835% of test data
```

1.5.4 Data Preprocessing

```
In [5]: #function to get the input and output
        def get_allocate_value(train_top,test_top,dev_top):
            train_list=train_top.index.tolist()
```

```
    test_list=test_top.index.tolist()
    dev_list=dev_top.index.tolist()
    x_train=train.loc[train['family_id'].isin(train_list)]
    x_test=test.loc[test['family_id'].isin(test_list)]
    x_dev=dev.loc[dev['family_id'].isin(dev_list)]
    y_train=x_train['family_accession'].values
    x_train=x_train['sequence']
    y_test=x_test['family_accession'].values
    x_test=x_test['sequence']

    y_dev=x_dev['family_accession'].values
    x_dev=x_dev['sequence']
    return x_train,x_test,x_dev,y_train,y_test,y_dev

#function to onehotencode the output
def encode(y_train,y_test,y_dev):
    lb = LabelEncoder()
    y_train = lb.fit_transform(y_train)
    y_test=lb.transform(y_test)
    y_dev = lb.transform(y_dev)
    y_train=np.array(y_train)
    y_test=np.array(y_test)
    y_dev=np.array(y_dev)
    # Transform labels to one-hot
    lb = OneHotEncoder()
    y_train = lb.fit_transform(y_train.reshape(-1, 1))
    y_test=lb.transform(y_test.reshape(-1, 1))
    y_dev = lb.transform(y_dev.reshape(-1, 1))
    return y_train,y_test,y_dev

#function to convert the one letter amino acid into 3 letter and seperate them with a
def preprocess(x_train,x_test,x_dev):
    preprocess_train=[]
    for i in tqdm(x_train.values):
        g=seq3(i)
        preprocess_train.append(' '.join([g[i:i+3] for i in range(0, len(g), 3)]))

    preprocess_test=[]
    for i in tqdm(x_test.values):
        e=seq3(i)
        preprocess_test.append(' '.join([e[i:i+3] for i in range(0, len(e), 3)]))

    preprocess_dev=[]
    for i in tqdm(x_dev.values):
        f=seq3(i)
        preprocess_dev.append(' '.join([f[i:i+3] for i in range(0, len(f), 3)]))

    return preprocess_train, preprocess_test, preprocess_dev
```

1.6 One Hot Encoding

We will one hot encode the input sequence into L*20 array such that each column represents one hot encoding of each amino acid and padding with zeroes

```
In [8]: #getting all the data

        train_top=train.groupby('family_id').size().sort_values(ascending=False).head(1000)
        dev_top=dev.groupby('family_id').size().sort_values(ascending=False).head(800)
        test_top=test.groupby('family_id').size().sort_values(ascending=False).head(800)

        x_train,x_test,x_dev,y_train,y_test,y_dev= get_allocate_value(train_top,test_top,dev_to
        y_train,y_test,y_dev=encode(y_train,y_test,y_dev)
        preprocess_train, preprocess_test, preprocess_dev= preprocess(x_train,x_test,x_dev)
```

```
100%|| 439493/439493 [00:28<00:00, 15521.62it/s]
100%|| 48262/48262 [00:03<00:00, 15432.02it/s]
100%|| 48262/48262 [00:03<00:00, 15736.93it/s]
```

```
In [9]: # Fit one hot encoding on train set
        l=[]
        for g in tqdm(x_train):
            z=(' '.join([g[i:i+1] for i in range(0, len(g), 1)]))
            f=z.split()
            l.append(f)

        corpus=[]
        for x in l:
            for c in x:
                corpus.append(c)

        lb = OneHotEncoder(sparse=False)
        gg=lb.fit(np.array(corpus).reshape(-1, 1))
```

```
100%|| 439493/439493 [00:15<00:00, 28881.03it/s]
```

```
In [12]: #One hot encoding of train,test and dev set
         c=0
         train_encod=[]
         dev_encod=[]
         test_encod=[]
         from tqdm.auto import tqdm
         for train in tqdm(x_train):
             z=(' '.join([train[i:i+1] for i in range(0, len(train), 1)]))
             f=z.split()
             train_p=lb.transform(np.array(f).reshape(-1, 1))
             train_p=sequence.pad_sequences(train_p.T, maxlen=400,padding='post')
```

```
            train_p=train_p.T
            train_p=sequence.pad_sequences(train_p, maxlen=20)

              #gg=gg.T
            train_encod.append(train_p[:,:20].tolist())

        for test in tqdm(x_test):
            z=(' '.join([test[i:i+1] for i in range(0, len(test), 1)]))
            f=z.split()
            test_p=lb.transform(np.array(f).reshape(-1, 1))
            test_p=sequence.pad_sequences(test_p.T, maxlen=400,padding='post')
            test_p=test_p.T
            test_p=sequence.pad_sequences(test_p, maxlen=20)
            test_encod.append(test_p[:,:20].tolist())

        for dev in tqdm(x_dev):
            z=(' '.join([dev[i:i+1] for i in range(0, len(dev), 1)]))
            f=z.split()
            dev_p=lb.transform(np.array(f).reshape(-1, 1))
            dev_p=sequence.pad_sequences(dev_p.T, maxlen=400,padding='post')
            dev_p=dev_p.T
            dev_p=sequence.pad_sequences(dev_p, maxlen=20)
            dev_encod.append(dev_p[:,:20].tolist())
          #x_in=sequence.pad_sequences(x_in[0], maxlen=200)
```

```
HBox(children=(IntProgress(value=0, max=439493), HTML(value='')))
```

```
HBox(children=(IntProgress(value=0, max=48262), HTML(value='')))
```

```
HBox(children=(IntProgress(value=0, max=48262), HTML(value='')))
```

```
In [38]: print('The number of rows are:',len(train_encod[0]))
         print('The number of columns are:',len(train_encod[0][0]))
         print('The number of datapoints are:',len(train_encod))
```

```
The number of rows are: 400
The number of columns are: 20
The number of datapoints are: 439493
```

The input contains 439,493 lists with each list containing 400*20 shaped list corresponding to output variable

```
In [13]: output_dim=1000
         input_dim=(100,20)
         batch_size=64
         epoch=1
```

```
In [12]: #https://www.kaggle.com/meownoid/tiny-resnet-with-keras-99-314
         #https://machinelearningmastery.com/how-to-implement-major-architecture-innovations-f

         from keras.layers import Dense, Conv1D
         # example of a CNN model with an identity or projection residual module
         from keras.models import Model
         from keras.layers import Input
         from keras.layers import Activation
         from keras.layers import Conv2D
         from keras.layers import MaxPooling2D
         from keras.layers import add
         from keras.utils import plot_model

         # function for creating an identity or projection residual module
         def residual_module(layer_in, n_filters):
             merge_input = layer_in
             # check if the number of filters needs to be increase, assumes channels last form
             if layer_in.shape[-1] != n_filters:
                 merge_input = Conv1D(n_filters, kernel_size=5, padding='same', activation='re

             x=BatchNormalization()(layer_in)
             x = Activation('relu')(x)
             #conv1
             conv1 = Conv1D(n_filters, kernel_size=5, padding='same', activation='relu', kerne
             x=BatchNormalization()(conv1)

             x = Activation('relu')(x)
             # conv2
             conv2 = Conv1D(n_filters,  kernel_size=5, padding='same', activation='linear', ke
             # add filters, assumes filters/channels last
             layer_out = add([conv2, merge_input])
             # activation function
             layer_out = Activation('relu')(layer_out)
             return layer_out


         visible = Input(shape=(100,20))
         x = Conv1D(kernel_size=3, filters=32, strides=1, padding='same')(visible)
         x = BatchNormalization()(x)
         x = Activation('relu')(x)
```

```
x = residual_module(x,128)
x = BatchNormalization()(x)
x = Activation('relu')(x)

# dropout for more robust learning
x = Dropout(0.2)(x)
x=Flatten()(x)
# last softmax layer
x = Dense(units=1000)(x)
x = Activation('softmax')(x)

#layer = residual_module(x, 32)
model = Model(inputs=visible, outputs=x)

model.summary()
# plot model architecture
plot_model(model, show_shapes=True, to_file='residual_module.png')
```

```
______________________________________________________________________________________________
Layer (type)                    Output Shape         Param #     Connected to
==============================================================================================
input_1 (InputLayer)            (None, 100, 20)      0
______________________________________________________________________________________________
conv1d_1 (Conv1D)               (None, 100, 32)      1952        input_1[0][0]
______________________________________________________________________________________________
batch_normalization_1 (BatchNor (None, 100, 32)      128         conv1d_1[0][0]
______________________________________________________________________________________________
activation_1 (Activation)       (None, 100, 32)      0           batch_normalization_1[0][0]
______________________________________________________________________________________________
batch_normalization_2 (BatchNor (None, 100, 32)      128         activation_1[0][0]
______________________________________________________________________________________________
activation_2 (Activation)       (None, 100, 32)      0           batch_normalization_2[0][0]
______________________________________________________________________________________________
conv1d_3 (Conv1D)               (None, 100, 128)     20608       activation_2[0][0]
______________________________________________________________________________________________
batch_normalization_3 (BatchNor (None, 100, 128)     512         conv1d_3[0][0]
______________________________________________________________________________________________
activation_3 (Activation)       (None, 100, 128)     0           batch_normalization_3[0][0]
______________________________________________________________________________________________
conv1d_4 (Conv1D)               (None, 100, 128)     82048       activation_3[0][0]
______________________________________________________________________________________________
conv1d_2 (Conv1D)               (None, 100, 128)     20608       activation_1[0][0]
______________________________________________________________________________________________
add_1 (Add)                     (None, 100, 128)     0           conv1d_4[0][0]
                                                                 conv1d_2[0][0]
______________________________________________________________________________________________
activation_4 (Activation)       (None, 100, 128)     0           add_1[0][0]
```

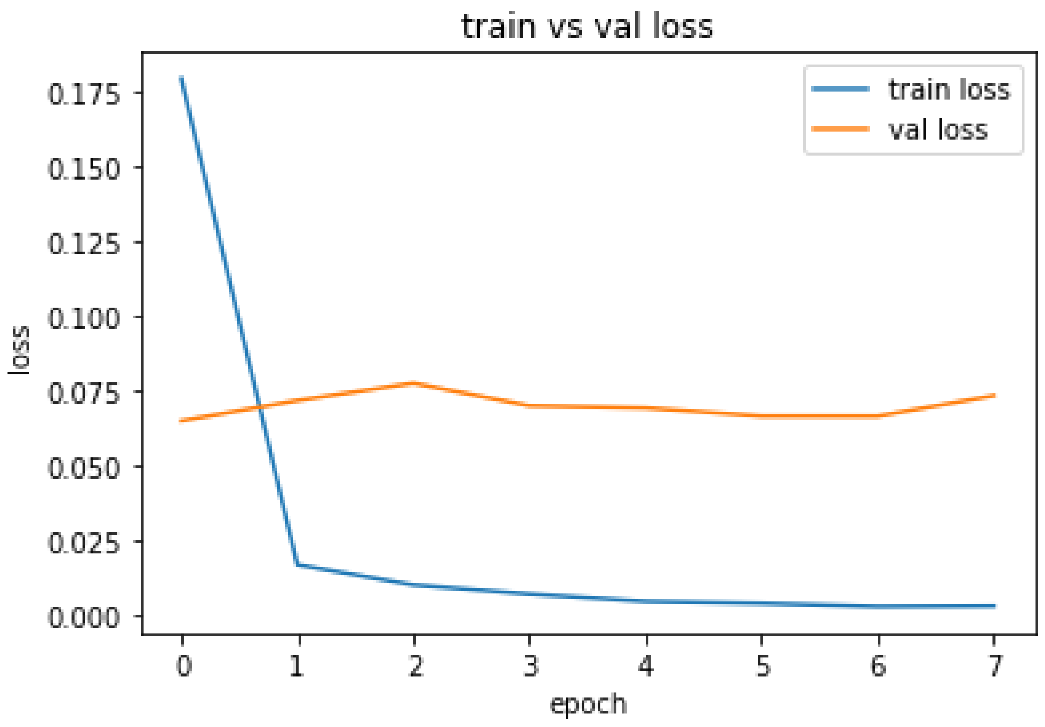
```
________________________________________________________________________________________________
batch_normalization_4 (BatchNor (None, 100, 128)     512         activation_4[0][0]
________________________________________________________________________________________________
activation_5 (Activation)       (None, 100, 128)     0           batch_normalization_4[0][0]
________________________________________________________________________________________________
dropout_1 (Dropout)             (None, 100, 128)     0           activation_5[0][0]
________________________________________________________________________________________________
flatten_1 (Flatten)             (None, 12800)        0           dropout_1[0][0]
________________________________________________________________________________________________
dense_1 (Dense)                 (None, 1000)         12801000    flatten_1[0][0]
________________________________________________________________________________________________
activation_6 (Activation)       (None, 1000)         0           dense_1[0][0]
================================================================================================
Total params: 12,927,496
Trainable params: 12,926,856
Non-trainable params: 640
________________________________________________________________________________________________
```

```
In [14]: #https://machinelearningmastery.com/how-to-stop-training-deep-neural-networks-at-the-
         #compiling and fitting the model
         model.compile(optimizer='adam',loss='categorical_crossentropy',metrics=['accuracy'])


         es = EarlyStopping(monitor='val_loss', mode='min', verbose=1, patience=7)
         mc = ModelCheckpoint('best_model_one_hot.h5', monitor='val_acc', mode='max', verbose=
         # fit model

         history = model.fit(np.array(train_encod),y_train,batch_size=128,epochs=15,verbose=1,
```

```
Train on 439493 samples, validate on 48262 samples
Epoch 1/15
439493/439493 [==============================] - 1235s 3ms/step - loss: 0.1795 - acc: 0.9650 -

Epoch 00001: val_acc improved from -inf to 0.98519, saving model to best_model_one_hot.h5
Epoch 2/15
439493/439493 [==============================] - 1238s 3ms/step - loss: 0.0170 - acc: 0.9963 -

Epoch 00002: val_acc improved from 0.98519 to 0.98560, saving model to best_model_one_hot.h5
Epoch 3/15
439493/439493 [==============================] - 1227s 3ms/step - loss: 0.0103 - acc: 0.9975 -

Epoch 00003: val_acc improved from 0.98560 to 0.98620, saving model to best_model_one_hot.h5
Epoch 4/15
439493/439493 [==============================] - 1225s 3ms/step - loss: 0.0072 - acc: 0.9982 -

Epoch 00004: val_acc improved from 0.98620 to 0.98701, saving model to best_model_one_hot.h5
Epoch 5/15
```

```
439493/439493 [==============================] - 1236s 3ms/step - loss: 0.0048 - acc: 0.9989 -

Epoch 00005: val_acc improved from 0.98701 to 0.98813, saving model to best_model_one_hot.h5
Epoch 6/15
439493/439493 [==============================] - 1236s 3ms/step - loss: 0.0041 - acc: 0.9991 -

Epoch 00006: val_acc improved from 0.98813 to 0.98856, saving model to best_model_one_hot.h5
Epoch 7/15
439493/439493 [==============================] - 1246s 3ms/step - loss: 0.0030 - acc: 0.9994 -

Epoch 00007: val_acc improved from 0.98856 to 0.98894, saving model to best_model_one_hot.h5
Epoch 8/15
439493/439493 [==============================] - 1241s 3ms/step - loss: 0.0032 - acc: 0.9993 -

Epoch 00008: val_acc did not improve from 0.98894
Epoch 00008: early stopping
```

```
In [15]: #plotting train and validation loss
         plt.plot(history.history['loss'], label='train loss')
         plt.plot(history.history['val_loss'], label='val loss')
         plt.title('train vs val loss')
         plt.xlabel('epoch')
         plt.ylabel('loss')
         plt.legend()
         plt.show()
```



```
In [16]: # evaluate
         test_acc = model.evaluate(np.array(test_encod),y_test, verbose=0)

         print('Test loss: %.3f' % ( test_acc[0]))
         print(' Test accuracy: %.3f' % (test_acc[1]))

Test loss: 0.076
 Test accuracy: 0.988
```

```
In [17]: test_pred=model.predict(np.array(test_encod))
         print('f1 score is ',f1_score(np.argmax(test_pred, axis=1), np.argmax(y_test, axis=1)

f1 score is  0.9877957813600763
```

1.7 k-mer Encoding

```
In [0]: #getting all the data

        train_top=train.groupby('family_id').size().sort_values(ascending=False).head(1000)
        dev_top=dev.groupby('family_id').size().sort_values(ascending=False).head(800)
        test_top=test.groupby('family_id').size().sort_values(ascending=False).head(800)

        x_train,x_test,x_dev,y_train,y_test,y_dev= get_allocate_value(train_top,test_top,dev_t
        y_train,y_test,y_dev=encode(y_train,y_test,y_dev)
        preprocess_train, preprocess_test, preprocess_dev= preprocess(x_train,x_test,x_dev)

100%|| 439493/439493 [00:26<00:00, 16396.71it/s]
100%|| 48262/48262 [00:02<00:00, 16516.85it/s]
100%|| 48262/48262 [00:02<00:00, 16511.98it/s]
```

```
In [0]: x_train.head()

Out[0]: 1    AGVPCSVKASEGYLFPLDRCFLFVTKPTLYIPYSEISSVVMSRTGG...
        2    IRHVLMNSPPGKLYDLVKDINILLGSSVSIQKILEEVLKDYNEKNY...
        3    MCIAIPGRIERIDYPIAIVDFKGLKKEVRIDLLENPQIGDYVLVHV...
        4    NIFHILWEDVDLEGVTFKPMGESISVQGDIHIFVLYEGEGENTPIR...
        5    VSPILQSLLDQLETTPAYILDQRMNIVGWNEAFSDVYGDYLYKGER...
        Name: sequence, dtype: object
```

1.8 MLP

Bigram

```
In [0]: #Bigram vectorization
        vectorizer = CountVectorizer(ngram_range=(0,2))
        X_train = vectorizer.fit_transform(preprocess_train)
        X_test = vectorizer.transform(preprocess_test)
        X_dev = vectorizer.transform(preprocess_dev)
        #print(vectorizer.get_feature_names())
```

```
In [201]: X_train[0]
```

```
Out[201]: <1x434 sparse matrix of type '<class 'numpy.int64'>'
                  with 70 stored elements in Compressed Sparse Row format>
```

```
In [0]: X_test.shape
```

```
Out[0]: (101536, 537)
```

```
In [0]: output_dim=1000
        input_dim=491
        batch_size=256
        epoch=20
```

```
In [0]: #building a model
        model = Sequential()

        model.add(Dense(512, input_dim=input_dim,activation='relu',kernel_initializer=RandomNo

        model.add(Dense(128,activation='relu',kernel_initializer=RandomNormal(mean=0.0, stddev
        model.add(BatchNormalization())
        model.add(Dropout(0.2))
        model.add(Dense(64,activation='relu',kernel_initializer=RandomNormal(mean=0.0, stddev=
        model.add(Dense(1000,activation='softmax'))
        model.summary()
```

```
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_2 (Dense)              (None, 512)               251904
_________________________________________________________________
dense_3 (Dense)              (None, 128)               65664
_________________________________________________________________
batch_normalization_1 (Batch (None, 128)               512
_________________________________________________________________
dropout_1 (Dropout)          (None, 128)               0
_________________________________________________________________
dense_4 (Dense)              (None, 64)                8256
_________________________________________________________________
dense_5 (Dense)              (None, 1000)              65000
=================================================================
Total params: 391,336
```

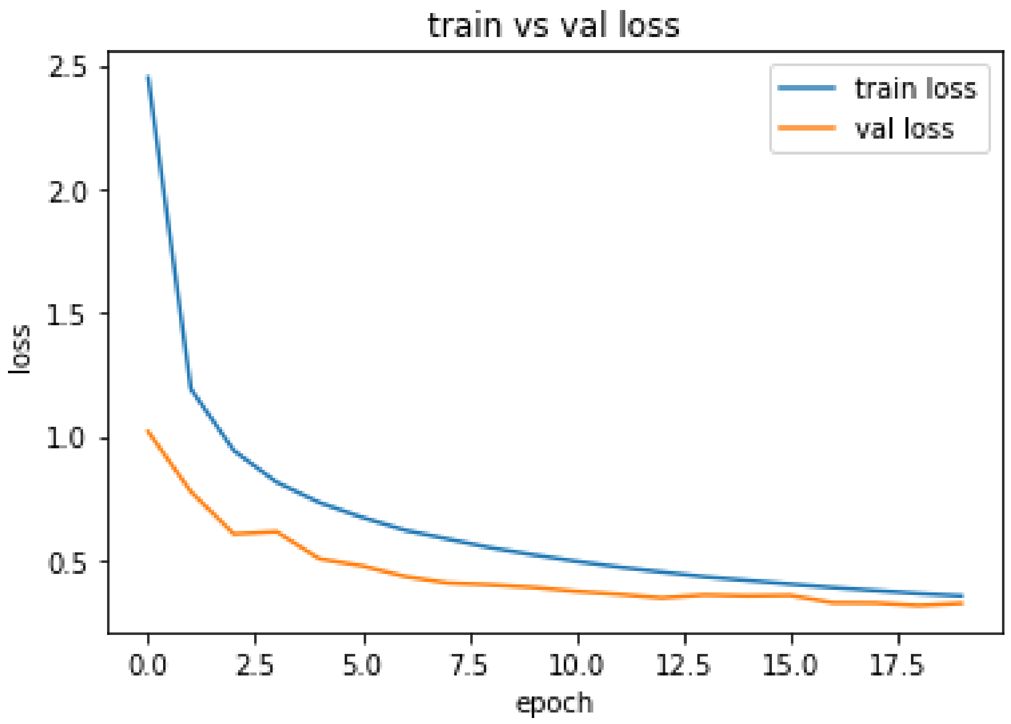
```
Trainable params: 391,080
Non-trainable params: 256
_________________________________________________________________
```

```
In [0]: #https://machinelearningmastery.com/how-to-stop-training-deep-neural-networks-at-the-r
        #compiling and fitting the model
        model.compile(optimizer='adam',loss='categorical_crossentropy',metrics=['accuracy'])


        es = EarlyStopping(monitor='val_loss', mode='min', verbose=1, patience=4)
        mc = ModelCheckpoint('best_model_bow_bigram.h5', monitor='val_acc', mode='max', verbose
        # fit model
        history = model.fit(X_train,y_train,batch_size=batch_size,epochs=epoch,verbose=1,valida

        # plot training history
        plt.plot(history.history['loss'], label='train loss')
        plt.plot(history.history['val_loss'], label='val loss')
        plt.title('train vs val loss')
        plt.xlabel('epoch')
        plt.ylabel('loss')
        plt.legend()
        plt.show()
```

```
Train on 439493 samples, validate on 48262 samples
Epoch 1/20
439493/439493 [==============================] - 21s 48us/step - loss: 2.4501 - acc: 0.4631 - v

Epoch 00001: val_acc improved from -inf to 0.74437, saving model to best_model_bow_bigram.h5
Epoch 2/20
439493/439493 [==============================] - 16s 37us/step - loss: 1.1906 - acc: 0.6938 - v

Epoch 00002: val_acc improved from 0.74437 to 0.80063, saving model to best_model_bow_bigram.h5
Epoch 3/20
439493/439493 [==============================] - 17s 38us/step - loss: 0.9418 - acc: 0.7529 - v

Epoch 00003: val_acc improved from 0.80063 to 0.84230, saving model to best_model_bow_bigram.h5
Epoch 4/20
439493/439493 [==============================] - 19s 42us/step - loss: 0.8146 - acc: 0.7839 - v

Epoch 00004: val_acc did not improve from 0.84230
Epoch 5/20
439493/439493 [==============================] - 18s 42us/step - loss: 0.7320 - acc: 0.8036 - v

Epoch 00005: val_acc improved from 0.84230 to 0.86457, saving model to best_model_bow_bigram.h5
Epoch 6/20
439493/439493 [==============================] - 17s 40us/step - loss: 0.6719 - acc: 0.8189 - v
```

```
Epoch 00006: val_acc improved from 0.86457 to 0.87267, saving model to best_model_bow_bigram.h5
Epoch 7/20
439493/439493 [==============================] - 18s 41us/step - loss: 0.6199 - acc: 0.8313 - v

Epoch 00007: val_acc improved from 0.87267 to 0.88424, saving model to best_model_bow_bigram.h5
Epoch 8/20
439493/439493 [==============================] - 17s 39us/step - loss: 0.5843 - acc: 0.8413 - v

Epoch 00008: val_acc improved from 0.88424 to 0.89149, saving model to best_model_bow_bigram.h5
Epoch 9/20
439493/439493 [==============================] - 18s 41us/step - loss: 0.5491 - acc: 0.8493 - v

Epoch 00009: val_acc improved from 0.89149 to 0.89250, saving model to best_model_bow_bigram.h5
Epoch 10/20
439493/439493 [==============================] - 18s 41us/step - loss: 0.5202 - acc: 0.8567 - v

Epoch 00010: val_acc improved from 0.89250 to 0.89553, saving model to best_model_bow_bigram.h5
Epoch 11/20
439493/439493 [==============================] - 18s 42us/step - loss: 0.4940 - acc: 0.8632 - v

Epoch 00011: val_acc improved from 0.89553 to 0.89938, saving model to best_model_bow_bigram.h5
Epoch 12/20
439493/439493 [==============================] - 18s 41us/step - loss: 0.4708 - acc: 0.8694 - v

Epoch 00012: val_acc improved from 0.89938 to 0.90290, saving model to best_model_bow_bigram.h5
Epoch 13/20
439493/439493 [==============================] - 18s 41us/step - loss: 0.4507 - acc: 0.8739 - v

Epoch 00013: val_acc improved from 0.90290 to 0.90491, saving model to best_model_bow_bigram.h5
Epoch 14/20
439493/439493 [==============================] - 15s 33us/step - loss: 0.4313 - acc: 0.8793 - v

Epoch 00014: val_acc did not improve from 0.90491
Epoch 15/20
439493/439493 [==============================] - 14s 33us/step - loss: 0.4167 - acc: 0.8828 - v

Epoch 00015: val_acc did not improve from 0.90491
Epoch 16/20
439493/439493 [==============================] - 14s 32us/step - loss: 0.4019 - acc: 0.8865 - v

Epoch 00016: val_acc improved from 0.90491 to 0.90508, saving model to best_model_bow_bigram.h5
Epoch 17/20
439493/439493 [==============================] - 14s 33us/step - loss: 0.3877 - acc: 0.8900 - v

Epoch 00017: val_acc improved from 0.90508 to 0.91204, saving model to best_model_bow_bigram.h5
Epoch 18/20
439493/439493 [==============================] - 14s 33us/step - loss: 0.3755 - acc: 0.8929 - v
```

```
Epoch 00018: val_acc improved from 0.91204 to 0.91225, saving model to best_model_bow_bigram.h5
Epoch 19/20
439493/439493 [==============================] - 14s 33us/step - loss: 0.3638 - acc: 0.8965 - v

Epoch 00019: val_acc improved from 0.91225 to 0.91561, saving model to best_model_bow_bigram.h5
Epoch 20/20
439493/439493 [==============================] - 14s 32us/step - loss: 0.3543 - acc: 0.8987 - v

Epoch 00020: val_acc did not improve from 0.91561
```



```
In [0]: test_pred=model.predict(X_test)
        print('f1 score is ',f1_score(np.argmax(test_pred, axis=1), np.argmax(y_test, axis=1),a

f1 score is  0.9092660892627741
```

```
In [0]: # load the saved model
        #saved_model = load_model('best_model_bow_bigram.h5')
        # evaluate the model
        train_acc = model.evaluate(X_train,y_train, verbose=0)
        test_acc = model.evaluate(X_test,y_test, verbose=0)
        dev_acc = model.evaluate(X_dev,y_dev, verbose=0)
        print('Train loss: %.3f, Test loss: %.3f, Dev loss : %3f' % (train_acc[0], test_acc[0]
        print('Train accuracy: %.3f, Test accuracy: %.3f, Dev accuracy : %3f' % (train_acc[1],
Train loss: 0.190, Test loss: 0.336, Dev loss : 0.324030
Train accuracy: 0.946, Test accuracy: 0.909, Dev accuracy : 0.911732
```

Trigram

```
In [0]: #Trigram vectorization of the dataset
        vectorizer = CountVectorizer(ngram_range=(1,3))
        X_train = vectorizer.fit_transform(preprocess_train)
        X_test = vectorizer.transform(preprocess_test)
        X_dev = vectorizer.transform(preprocess_dev)
```

```
In [0]: X_train.shape
```

```
Out[0]: (439493, 9085)
```

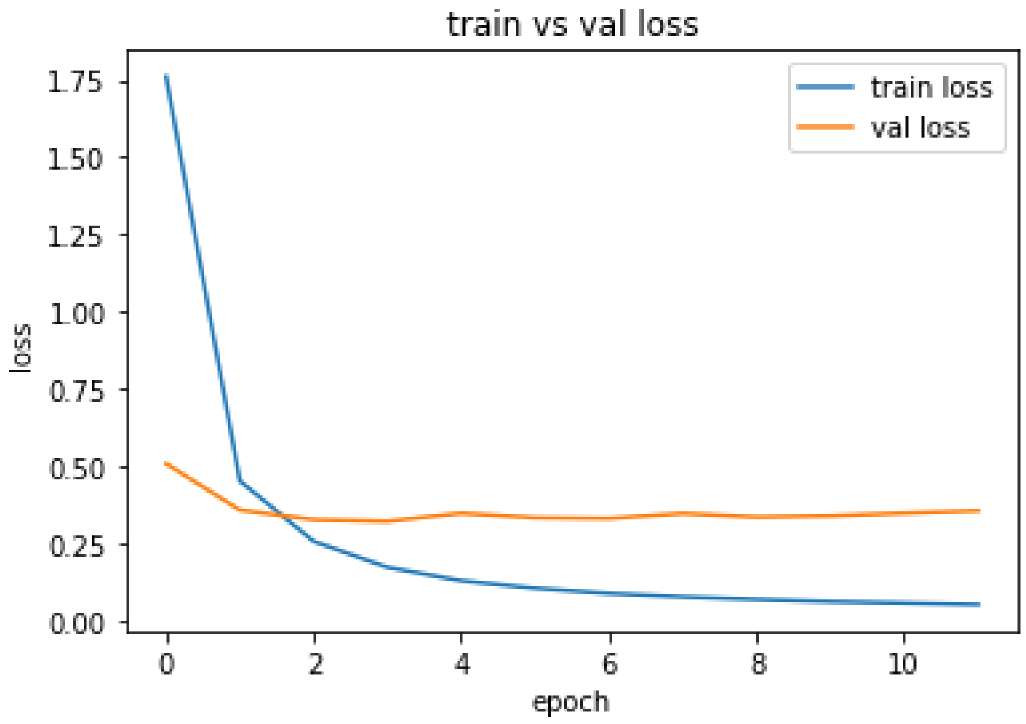
```
In [0]: output_dim=1000
        input_dim=9085
        batch_size=256
        epoch=20
```

```
In [0]: #building the model

        model = Sequential()

        model.add(Dense(512, input_dim=input_dim,activation='relu',kernel_initializer=RandomNo

        model.add(Dense(128,activation='relu',kernel_initializer=RandomNormal(mean=0.0, stddev=
        model.add(BatchNormalization())
        model.add(Dropout(0.2))
        model.add(Dense(64,activation='relu',kernel_initializer=RandomNormal(mean=0.0, stddev=
        model.add(Dense(1000,activation='softmax'))
        model.summary()
```

```
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_14 (Dense)             (None, 512)               4652032
_________________________________________________________________
dense_15 (Dense)             (None, 128)               65664
_________________________________________________________________
batch_normalization_4 (Batch (None, 128)               512
_________________________________________________________________
dropout_4 (Dropout)          (None, 128)               0
_________________________________________________________________
dense_16 (Dense)             (None, 64)                8256
_________________________________________________________________
dense_17 (Dense)             (None, 1000)              65000
=================================================================
Total params: 4,791,464
Trainable params: 4,791,208
Non-trainable params: 256
_________________________________________________________________
```

```
In [0]: #compiling and fitting the model
        model.compile(optimizer='adam',loss='categorical_crossentropy',metrics=['accuracy'])

        es = EarlyStopping(monitor='val_loss', mode='min', verbose=1, patience=8)
        mc = ModelCheckpoint('best_model_bow_trigram.h5', monitor='val_acc', mode='max', verbos
        # fit model
        history = model.fit(X_train,y_train,batch_size=batch_size,epochs=epoch,verbose=1,valida

        # plot training history
        plt.plot(history.history['loss'], label='train loss')
        plt.plot(history.history['val_loss'], label='val loss')
        plt.title('train vs val loss')
        plt.xlabel('epoch')
        plt.ylabel('loss')
        plt.legend()
        plt.show()
```

```
Train on 439493 samples, validate on 48262 samples
Epoch 1/20
439493/439493 [==============================] - 43s 99us/step - loss: 1.7611 - acc: 0.6335 - v

Epoch 00001: val_acc improved from -inf to 0.87118, saving model to best_model_bow_trigram.h5
Epoch 2/20
439493/439493 [==============================] - 42s 95us/step - loss: 0.4523 - acc: 0.8790 - v

Epoch 00002: val_acc improved from 0.87118 to 0.90692, saving model to best_model_bow_trigram.h
Epoch 3/20
439493/439493 [==============================] - 42s 96us/step - loss: 0.2564 - acc: 0.9274 - v

Epoch 00003: val_acc improved from 0.90692 to 0.91728, saving model to best_model_bow_trigram.h
Epoch 4/20
439493/439493 [==============================] - 43s 97us/step - loss: 0.1723 - acc: 0.9486 - v

Epoch 00004: val_acc improved from 0.91728 to 0.92110, saving model to best_model_bow_trigram.h
Epoch 5/20
439493/439493 [==============================] - 42s 96us/step - loss: 0.1288 - acc: 0.9608 - v

Epoch 00005: val_acc did not improve from 0.92110
Epoch 6/20
439493/439493 [==============================] - 42s 96us/step - loss: 0.1044 - acc: 0.9676 - v

Epoch 00006: val_acc improved from 0.92110 to 0.92646, saving model to best_model_bow_trigram.h
Epoch 7/20
439493/439493 [==============================] - 42s 97us/step - loss: 0.0875 - acc: 0.9728 - v

Epoch 00007: val_acc improved from 0.92646 to 0.92769, saving model to best_model_bow_trigram.h
Epoch 8/20
439493/439493 [==============================] - 41s 94us/step - loss: 0.0764 - acc: 0.9762 - v

Epoch 00008: val_acc did not improve from 0.92769
Epoch 9/20
439493/439493 [==============================] - 42s 96us/step - loss: 0.0683 - acc: 0.9788 - v

Epoch 00009: val_acc improved from 0.92769 to 0.92854, saving model to best_model_bow_trigram.h
Epoch 10/20
439493/439493 [==============================] - 42s 96us/step - loss: 0.0613 - acc: 0.9810 - v

Epoch 00010: val_acc improved from 0.92854 to 0.93177, saving model to best_model_bow_trigram.h
Epoch 11/20
439493/439493 [==============================] - 42s 96us/step - loss: 0.0566 - acc: 0.9826 - v

Epoch 00011: val_acc did not improve from 0.93177
Epoch 12/20
439493/439493 [==============================] - 42s 96us/step - loss: 0.0516 - acc: 0.9842 - v

Epoch 00012: val_acc did not improve from 0.93177
Epoch 00012: early stopping
```



```
In [0]: #saved_model = load_model('best_model_bow_trigram.h5')
        #train_pred=saved_model.predict(X_train)
        test_pred=model.predict(X_test)
        print('f1 score is ',f1_score(np.argmax(test_pred, axis=1), np.argmax(y_test, axis=1),a
```

```
f1 score is  0.9308980150014504
```

```
In [0]: # load the saved model

        # evaluate the model
        train_acc = model.evaluate(X_train,y_train, verbose=0)
        test_acc = model.evaluate(X_test,y_test, verbose=0)
        dev_acc = model.evaluate(X_dev,y_dev, verbose=0)
        print('Train loss: %.3f, Test loss: %.3f, Dev loss : %3f' % (train_acc[0], test_acc[0]
        print('Train accuracy: %.3f, Test accuracy: %.3f, Dev accuracy : %3f' % (train_acc[1],
```

```
Train loss: 0.012, Test loss: 0.352, Dev loss : 0.355531
Train accuracy: 0.997, Test accuracy: 0.931, Dev accuracy : 0.930919
```

1.9 LSTM

```
In [0]: train_top=train.groupby('family_id').size().sort_values(ascending=False).head(1000)

        dev_top=dev.groupby('family_id').size().sort_values(ascending=False).head(800)

        test_top=test.groupby('family_id').size().sort_values(ascending=False).head(800)
```

```
In [0]: x_train,x_test,x_dev,y_train,y_test,y_dev= get_allocate_value(train_top,test_top,dev_t
        y_train,y_test,y_dev=encode(y_train,y_test,y_dev)
        preprocess_train, preprocess_test, preprocess_dev= preprocess(x_train,x_test,x_dev)
```

```
100%|| 439493/439493 [00:28<00:00, 15393.66it/s]
100%|| 48262/48262 [00:03<00:00, 15711.97it/s]
100%|| 48262/48262 [00:03<00:00, 15777.79it/s]
```

```
In [0]: vocab=[]

        for sent in tqdm(preprocess_train):
            words=sent.split(" ")
            vocab.append(words)

        vocab_all=[]
        for a in vocab:
            for x in a:
                vocab_all.append(x)
        vocab_all=set(vocab_all)
        # initialising all words with 0
        vocabulary=dict([(x,0) for x in vocab_all])

100%|| 439493/439493 [00:09<00:00, 47442.20it/s]
```

```
In [0]: #counting the occurence of each word
        count=0
        for sent in tqdm(preprocess_train):

            words=sent.split(" ")

            for x in words:
                if x in vocabulary.keys():
                    vocabulary[x]+=1

100%|| 439493/439493 [00:27<00:00, 15911.86it/s]
```

```
In [0]: vocabulary

Out[0]: {'Ala': 5988777,
         'Arg': 3609908,
         'Asn': 2433797,
         'Asp': 3576954,
         'Asx': 6,
         'Cys': 851185,
         'Gln': 2220574,
         'Glu': 4109154,
         'Gly': 5052648,
         'His': 1410422,
         'Ile': 4262868,
         'Leu': 6592761,
         'Lys': 3410226,
         'Met': 1510065,
         'Phe': 2698086,
         'Pro': 2779165,
         'Pyl': 1,
         'Sec': 7,
         'Ser': 3794491,
         'Thr': 3502984,
         'Trp': 790541,
         'Tyr': 2069051,
         'Val': 4916553,
         'Xaa': 410}
```

```
In [0]: # converting into dataframe
        vocab_df= pd.DataFrame(list(vocabulary.items()), columns=['words', 'count'])
        #sorting and getting the indices
        vocab_df=vocab_df.sort_values(by='count',ascending=False)
        top_vocab_df=vocab_df
        top_vocab_df=top_vocab_df.reset_index()

        vocab_dict={}
        top_vocab_df.head()
```

```
Out[0]:    index words    count
        0     12   Leu  6592761
        1     22   Ala  5988777
        2     13   Gly  5052648
        3     10   Val  4916553
        4     21   Ile  4262868
```

```
In [0]: #converting sentences to list of indexes
        vocab_dict=dict(zip(top_vocab_df['words'],top_vocab_df.index))
        count=0
        all_words_list=[]
        all_words_set=[]
        train_vocab=[]
        all_words_list=top_vocab_df['words'].tolist()
        all_words_set=set(all_words_list)
        for sent in tqdm(preprocess_train):
            sent_index=[]
           # print(sent)
            i=0
            word=sent.split(" ")

            for a in word:
                if a in all_words_set:
                    sent_index.append(vocab_dict[a])
            train_vocab.append(sent_index)
```

```
100%|| 439493/439493 [00:23<00:00, 18479.62it/s]
```

```
In [0]: #similary converting dev and test into list of indices
        dev_vocab=[]
        for sent in tqdm(preprocess_dev):
            sent_index=[]
           # print(sent)
            i=0
            word=sent.split(" ")

            for a in word:
                if a in all_words_set:
                    sent_index.append(vocab_dict[a])
            dev_vocab.append(sent_index)


        test_vocab=[]
        for sent in tqdm(preprocess_test):
            sent_index=[]
           # print(sent)
            i=0
            word=sent.split(" ")

            for a in word:
                if a in all_words_set:
                    sent_index.append(vocab_dict[a])
            test_vocab.append(sent_index)
```

```
100%|| 48262/48262 [00:02<00:00, 20993.15it/s]
100%|| 48262/48262 [00:04<00:00, 11200.25it/s]
```

```
In [0]: #padding with 0

        train_vocab = sequence.pad_sequences(train_vocab, maxlen=max_review_length)
        test_vocab = sequence.pad_sequences(test_vocab, maxlen=max_review_length)
        dev_vocab = sequence.pad_sequences(dev_vocab, maxlen=max_review_length)
```

```
In [0]: embedding_vecor_length = 32
        model = Sequential()
        model.add(Embedding(5000, embedding_vecor_length, input_length=max_review_length))
        model.add(LSTM(100))
        model.add(Dense(1000, activation='softmax'))
        model.compile(loss='categorical_crossentropy', optimizer='adam', metrics=['accuracy'])
        print(model.summary())
```

```
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
embedding_1 (Embedding)      (None, 100, 32)           160000
_________________________________________________________________
lstm_1 (LSTM)                (None, 100)               53200
_________________________________________________________________
dense_18 (Dense)             (None, 1000)              101000
=================================================================
Total params: 314,200
Trainable params: 314,200
Non-trainable params: 0
_________________________________________________________________
```

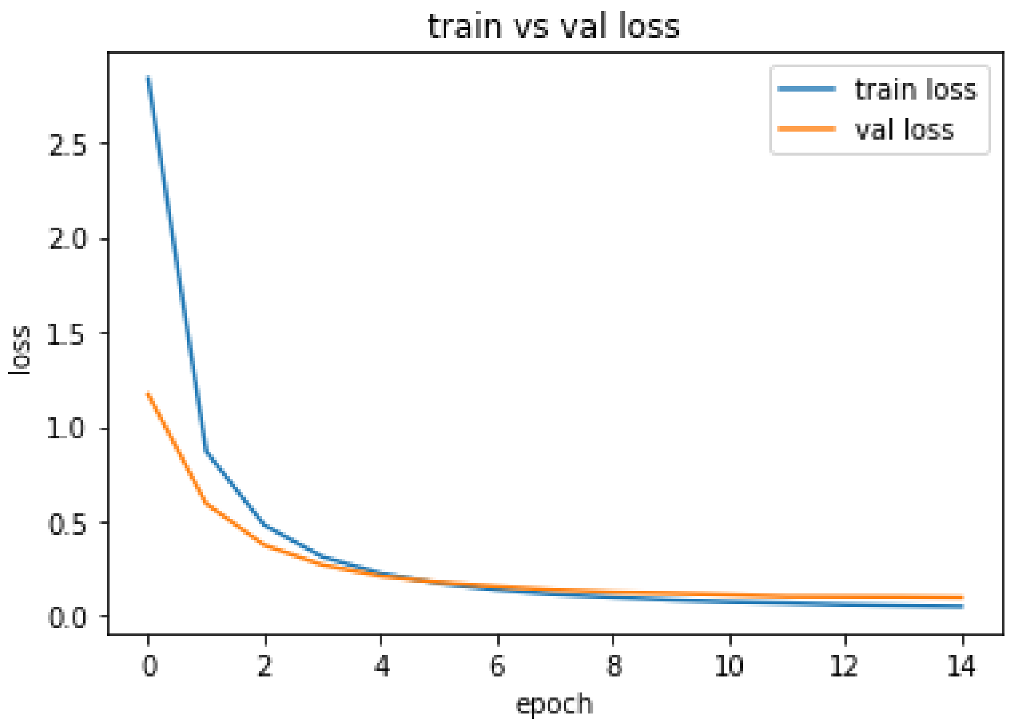
```
None
```

```
In [0]: es = EarlyStopping(monitor='val_loss', mode='min', verbose=1, patience=7)
        mc = ModelCheckpoint('best_model_lstm.h5', monitor='val_acc', mode='max', verbose=1, sa
        # fit model
        history=model.fit(train_vocab, y_train, nb_epoch=15, batch_size=128,verbose=1,validatio
```

```
Train on 439493 samples, validate on 48262 samples
Epoch 1/15
439493/439493 [==============================] - 540s 1ms/step - loss: 2.8383 - acc: 0.4833 - v

Epoch 00001: val_acc improved from -inf to 0.75917, saving model to best_model_lstm.h5
Epoch 2/15
439493/439493 [==============================] - 538s 1ms/step - loss: 0.8680 - acc: 0.8158 - v

Epoch 00002: val_acc improved from 0.75917 to 0.87340, saving model to best_model_lstm.h5
Epoch 3/15
439493/439493 [==============================] - 536s 1ms/step - loss: 0.4799 - acc: 0.8950 - v

Epoch 00003: val_acc improved from 0.87340 to 0.91764, saving model to best_model_lstm.h5
Epoch 4/15
439493/439493 [==============================] - 536s 1ms/step - loss: 0.3126 - acc: 0.9304 - v

Epoch 00004: val_acc improved from 0.91764 to 0.93863, saving model to best_model_lstm.h5
Epoch 5/15
439493/439493 [==============================] - 536s 1ms/step - loss: 0.2241 - acc: 0.9493 - v

Epoch 00005: val_acc improved from 0.93863 to 0.95029, saving model to best_model_lstm.h5
Epoch 6/15
439493/439493 [==============================] - 541s 1ms/step - loss: 0.1717 - acc: 0.9609 - v

Epoch 00006: val_acc improved from 0.95029 to 0.95759, saving model to best_model_lstm.h5
Epoch 7/15
439493/439493 [==============================] - 526s 1ms/step - loss: 0.1373 - acc: 0.9689 - v

Epoch 00007: val_acc improved from 0.95759 to 0.96349, saving model to best_model_lstm.h5
Epoch 8/15
439493/439493 [==============================] - 530s 1ms/step - loss: 0.1138 - acc: 0.9743 - v

Epoch 00008: val_acc improved from 0.96349 to 0.96654, saving model to best_model_lstm.h5
Epoch 9/15
439493/439493 [==============================] - 531s 1ms/step - loss: 0.0981 - acc: 0.9775 - v

Epoch 00009: val_acc improved from 0.96654 to 0.96844, saving model to best_model_lstm.h5
Epoch 10/15
439493/439493 [==============================] - 533s 1ms/step - loss: 0.0841 - acc: 0.9808 - v
```

```
Epoch 00010: val_acc improved from 0.96844 to 0.97047, saving model to best_model_lstm.h5
Epoch 11/15
439493/439493 [==============================] - 533s 1ms/step - loss: 0.0737 - acc: 0.9835 - v

Epoch 00011: val_acc improved from 0.97047 to 0.97269, saving model to best_model_lstm.h5
Epoch 12/15
439493/439493 [==============================] - 533s 1ms/step - loss: 0.0670 - acc: 0.9848 - v

Epoch 00012: val_acc improved from 0.97269 to 0.97354, saving model to best_model_lstm.h5
Epoch 13/15
439493/439493 [==============================] - 538s 1ms/step - loss: 0.0587 - acc: 0.9866 - v

Epoch 00013: val_acc improved from 0.97354 to 0.97406, saving model to best_model_lstm.h5
Epoch 14/15
439493/439493 [==============================] - 537s 1ms/step - loss: 0.0535 - acc: 0.9878 - v

Epoch 00014: val_acc improved from 0.97406 to 0.97414, saving model to best_model_lstm.h5
Epoch 15/15
439493/439493 [==============================] - 534s 1ms/step - loss: 0.0488 - acc: 0.9888 - v

Epoch 00015: val_acc improved from 0.97414 to 0.97424, saving model to best_model_lstm.h5
```

```
In [0]:  #plotting train and validation loss
        plt.plot(history.history['loss'], label='train loss')
        plt.plot(history.history['val_loss'], label='val loss')
        plt.title('train vs val loss')
        plt.xlabel('epoch')
        plt.ylabel('loss')
        plt.legend()
        plt.show()
```



```
In [0]: # evaluate the model
        train_acc = model.evaluate(train_vocab, y_train, verbose=0)
        test_acc = model.evaluate(test_vocab,y_test, verbose=0)
        dev_acc = model.evaluate(dev_vocab,y_dev, verbose=0)
        print('Train loss: %.3f, Test loss: %.3f, Dev loss : %3f' % (train_acc[0], test_acc[0]
        print('Train accuracy: %.3f, Test accuracy: %.3f, Dev accuracy : %3f' % (train_acc[1],

Train loss: 0.041, Test loss: 0.102, Dev loss : 0.097211
Train accuracy: 0.991, Test accuracy: 0.973, Dev accuracy : 0.974245
```

```
In [0]: # load the saved model
        #saved_model = load_model('best_model_lstm.h5')
        test_pred=model.predict(test_vocab)
        print('f1 score is ',f1_score(np.argmax(test_pred, axis=1), np.argmax(y_test, axis=1),a

f1 score is  0.9732501761220007
```

1.10 Conclusion

Objective: Given the amino acid sequence of the protein domain, predict which class it belongs to.

1. We are given a dataset with Train, Test and Dev files containing 1086741, 126171, 126171 rows and 5 columns: family_id, sequence_name,sequence,family_accession,aligned_sequence

where family_accession is the output label consisting of 17929 classes and sequence is the input.
2. We visualize the train and test data and see that the train, test and dev have the same distribution, we perform data analysis and find the family with longest sequence length, most common family etc.
3. We see that the 1000 classes cover almost 40% of the dataset and also to reduce the time complexity, we only consider 1000 classes.
4. We take Recall and logloss as evaluation metric.
5. We Preprocess the data and check for null values or duplicates and one hot encode the output class. We featurize the data using one hot encoding and converting into L*20 array where each column represents one hot encoding of each amino acid.
6. We also featurize the data using BoW bigrams and Trigrams since the input is a sequence of values and apply a mlp and find that both the models have similar accuracy of 93%.
7. We implement the protCNN model given in the paper using resnets. We use early stopping to avoid overfitting and save the models.
8. Since it is a sequence, we use LSTM model and consider only 1500 most common output classes due to huge training time and pass the indices as input to the model and the accuracy improved to 97%.
9. ProtCNN model gives the highest accuracy of 98.889%.

```
In [21]: from prettytable import PrettyTable

         x=PrettyTable()

         x.field_names=['Algorithm','ngram range','Vectorizor','F1 score','Train Accuracy','De

         x.add_row(['PROTCNN','-','One Hot Encoding',0.987, 99.9, 98.9,98.8])
         x.add_row(['MLP',2,'BoW',.909,94.6,91.1,90.9])
         x.add_row(['MLP',3,'BoW', .9308,99.7,93.09,93.1])
         x.add_row(['LSTM ','-','-',.973,99.1,97.4,97.3])

         print(x)
```

```
+-----------+-------------+------------------+----------+----------------+--------------+------
| Algorithm | ngram range |    Vectorizor    | F1 score | Train Accuracy | Dev Accuracy | Test
+-----------+-------------+------------------+----------+----------------+--------------+------
|  PROTCNN  |      -      | One Hot Encoding |  0.987   |      99.9      |     98.9     |
|    MLP    |      2      |       BoW        |  0.909   |      94.6      |     91.1     |
|    MLP    |      3      |       BoW        |  0.9308  |      99.7      |    93.09     |
|   LSTM    |      -      |        -         |  0.973   |      99.1      |     97.4     |
+-----------+-------------+------------------+----------+----------------+--------------+------
```

```
In [0]:
```