

Particle detection, Case Study 6

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Abstract

The report uses deep learning model to identify particle producing collisions from background source and investigate the most appropriate tuning parameters for the model.

1 Introduction

The study of minute particles that make up matter and radiations is called High Energy Physics (HEP). The study is used to experiment and search for signatures of rare particles which is learned by using monte Carlo simulations of the decaying product that is caused by collision of these particles [2]. The creation of such high energy particle is done using particle accelerators.

The application of these high energy partials is producing rare medical isotopes for research and medical treatments or used in radio therapy. Development of new superconductor material has also been pushed due to this. Other applications are in the area of medical, security, computing, science etc. [3]

In this paper we use the dataset hosted by UCI machine learning repository [1] called HEPMASS dataset. We use various deep learning models as a binary classifier to predict if a collision results in a new particle or not.

2 Method

The large HEPMASS dataset that has labeled data of a collisions resulting in particle presence and its associated features was analyzed, scaled and used as training a series of deep neural network models. Various models were analyzed for their tuning parameters such as number of layers, number of nodes, batch size etc. to identify the best performing model using the accuracy score. The best identified model was than evaluated for f1 score, its confusion matrix (CM) and Receiver Operating Characteristics (ROC) / Area Under the Curve (AUC).

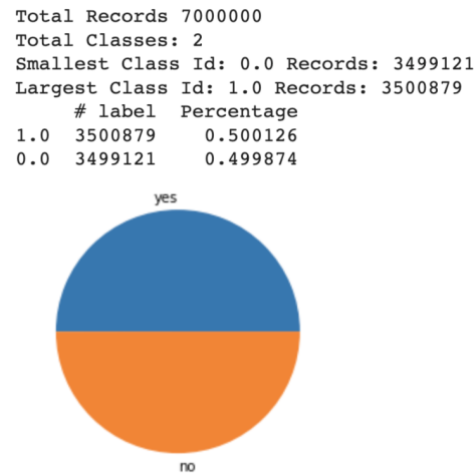
We first made a single stratified shuffle split of 90/10 % Where 90% was used for model building and 10% was our hold out for evaluation. The model building split was further split into 80/20 Train/Test split using the same strategy. The models were trained on the 80% train split and evaluated on the 20% test split. The CM and f1 statistics for the best model identified was carried out on the 10% holdout data of the best model identified.

2.1 Data

The data consists of 28 features of complex scientific data points for 7 million collisions and the binary target label that indicates if the collision resulted in a new particle or not. The histogram of most [5.1] variables show normal distribution with no missing values, also none of the features had any significant correlation between each other so all the rows and

features were included in our models. The features were scaled using standard scalar to be between 0 and 1. The target class was evenly distributed as shown in [Error! Reference source not found.]

Figure 1



[Table 1] below shows the final shape of the data used, 10% of the original data set was held back to evaluate the best model's performance and the remaining 90% was split into Train / Validation data using 80/20 split. Both the splits used a stratified split to maintain original class balance.

Table 1

Hold Out	Training	Validation
(700000, 28)	(5040000, 28)	(1260000, 28)
(700000,)	(5040000,)	(1260000,)

2.2 Models

The models that were evaluated were dense neural network consisting of 3 and 5 layers using relu activation and each was tuned using nodes varying between 400 to 800 at the first layer and 8 nodes at the layer before the output layer as it's a good recommendation of having the last layer around $\frac{1}{4}$ the number of features and nodes in the middle layers gradually decreasing by the fraction of the difference of first layer nodes and last layer nodes by number of layers $[(\text{num_start_nodes} - \text{num_end_nodes})/\text{num_layers}]$. The models also used two batch sizes namely 10000 and 20000. We used epoch size of 500 and an early stopping criterion was specified with a patience of 5 allowing the training to stop if there was no improvement seen in the validation score for 5 consecutive epochs.

3 Results

Table 2 shows each models parameter its total trainable parameters the number of epochs before early stopping kicks in and the model accuracy. The 5 layer in general performs better than 3 layers. In the 5-layer model the models with batch size of 10000 was slightly better than the ones

with 20000. We finally chose the model highlighted in red which had the highest accuracy of 88.5, batch of 10000 and nodes of (600, 452, 304, 156, 1)

Table 2

Model	Total Param	Epochs	Accuracy
Activation: relu layers: 3 nodes: 400, 204, 1 batch: 10000	93,609	70	87.81
Activation: relu layers: 3 nodes: 600, 304, 1 batch: 10000	200,409	68	88.13
Activation: relu layers: 3 nodes: 800, 404, 1 batch: 10000	347,209	86	88.36
Activation: relu layers: 3 nodes: 400, 204, 1 batch: 20000	93,609	45	85.61
Activation: relu layers: 3 nodes: 600, 304, 1 batch: 20000	200,409	18	83.62
Activation: relu layers: 3 nodes: 800, 404, 1 batch: 20000	347,209	34	85.55
Activation: relu layers: 5 nodes: 400, 302, 204, 106, 1 batch: 10000	216,351	49	88.17
Activation: relu layers: 5 nodes: 600, 452, 304, 156, 1 batch: 10000	474,501	66	88.5
Activation: relu layers: 5 nodes: 800, 602, 404, 206, 1 batch: 10000	832,651	61	88.4
Activation: relu layers: 5 nodes: 400, 302, 204, 106, 1 batch: 20000	216,351	89	88.1
Activation: relu layers: 5 nodes: 600, 452, 304, 156, 1 batch: 20000	474,501	89	88.22
Activation: relu layers: 5 nodes: 800, 602, 404, 206, 1 batch: 20000	832,651	50	87.75

3.1.1 Best Model Results

We evaluated the best performing model on the 10% holdout set. Figure 2 shows the drop in validation loss and increase in accuracy as the model trains, the model stops improving after 55 epochs. As seen in Figure 3 the over model f1 score 80%, the f1 score for class Yes is 82% and that for No is 77%, the AUC and Confusion Matrix (CM) are shown in Figure 4, the area under the curve is 95.6 %

Figure 2

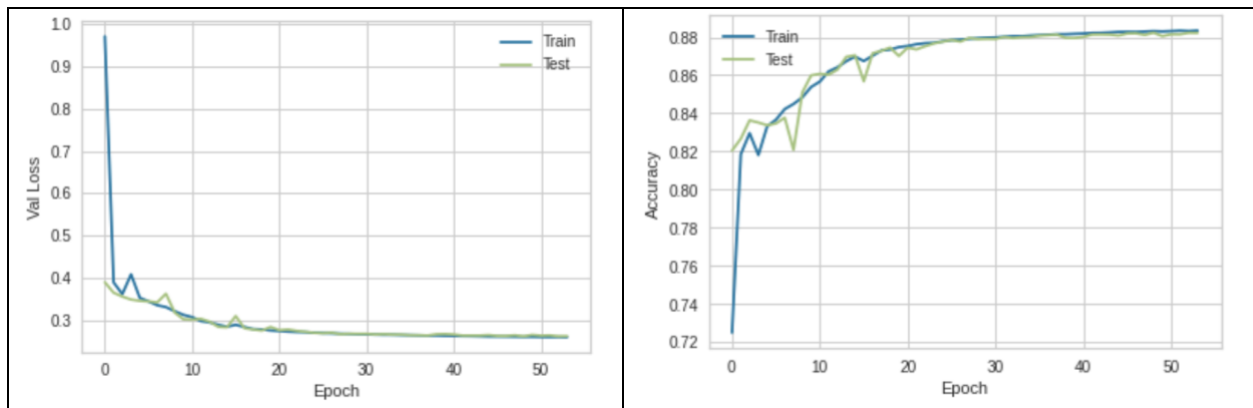
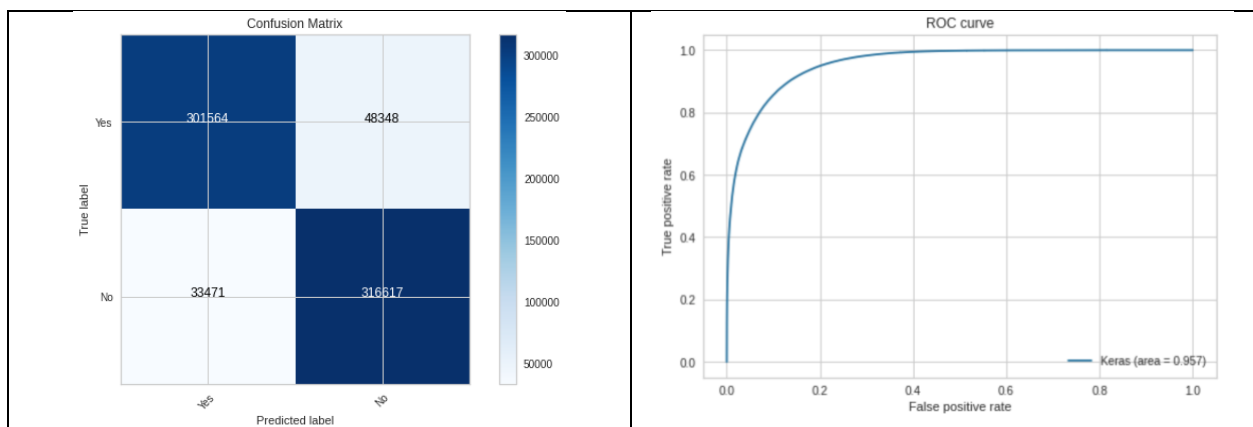


Figure 3

	precision	recall	f1-score	support
Yes	0.74	0.92	0.82	349912
No	0.89	0.67	0.77	350088
accuracy			0.80	700000
macro avg	0.81	0.80	0.79	700000
weighted avg	0.81	0.80	0.79	700000

Figure 4



4 Conclusion

The models were all generated using google colab using GPU and high memory to train the models in a reasonable time for this large dataset of 7 millions rows. Using 5-layers

and 474501 tunable parameters with batch size of 10000 we were able to train the model within 54 epochs with an early stopping of 5 epochs over validation loss. The best accuracy of the model was around 88.5% with an f1 score of 80%. The AUC derived using 50% threshold was 95.6%, we can potentially increase the threshold if there is a need to increase the potential of not missing a collision that results in a new particle. We can help the model train further by increasing the nodes (parameters) within the layers and tryout more tuning parameters such as learning rate, batch sizes and increasing the patience from 5 to 10 but that would need more resources.

5 Appendix

5.1 Code

Some of the output has been cleaned to reduce document.

```
import os
import email

#All Python module imports
#https://pandas.pydata.org/docs/user_guide/index.html#user-guide
import pandas as pd #Pandas Dataframe module
import numpy as np
from math import pi
#scikit learn

#https://scikit-learn.org/stable/modules/classes.html#module-sklearn.linear_model
import sklearn as skl

#https://seaborn.pydata.org
import seaborn as sns
import matplotlib.pyplot as plt
import matplotlib

import warnings
#Module for formating table for documentation
#https://pypi.org/project/tabulate/
from tabulate import tabulate

from IPython.display import display, Markdown
#Interactive mode
from IPython.core.interactiveshell import InteractiveShell
InteractiveShell.ast_node_interactivity = "all"
from IPython.display import Image

from sklearn.preprocessing import MinMaxScaler
```

```
from sklearn.feature_selection import SelectKBest, chi2
from sklearn.model_selection import StratifiedShuffleSplit
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LogisticRegression
from sklearn import metrics as mt
from sklearn.metrics import plot_confusion_matrix
from sklearn.model_selection import cross_val_score
from sklearn.metrics import classification_report
from sklearn.linear_model import LogisticRegression
from sklearn.svm import SVC
from sklearn.decomposition import PCA
from sklearn.metrics import confusion_matrix
from sklearn.metrics import f1_score, accuracy_score
from sklearn.model_selection import KFold, StratifiedKFold
from sklearn.model_selection import GridSearchCV as gridcv
from sklearn import preprocessing
from sklearn.model_selection import cross_validate
from sklearn.metrics import make_scorer
from sklearn.metrics import mean_squared_error
from sklearn.metrics import mean_absolute_error
from sklearn.metrics import r2_score
import pprint
import re
from sklearn.model_selection import cross_val_predict
from html.parser import HTMLParser
from bs4 import BeautifulSoup
import nltk
from nltk.corpus import stopwords
from sklearn.feature_extraction.text import TfidfVectorizer
from sklearn.metrics import roc_curve
from sklearn.metrics import roc_auc_score
from scipy.io import arff
from statsmodels.imputation import mice
import statsmodels as sm
from xgboost import XGBClassifier
from numpy import arange
from numpy import argmax
from sklearn.preprocessing import QuantileTransformer
import tensorflow as tf
import math
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense
from tensorflow.keras.wrappers.scikit_learn import KerasClassifier
from sklearn.preprocessing import MinMaxScaler
```

```

from sklearn.model_selection import train_test_split
from sklearn.model_selection import GridSearchCV, RandomizedSearchCV
print(tf.__version__)

import warnings
warnings.filterwarnings('ignore')
from yellowbrick.classifier import ROCAUC
import yellowbrick
print(yellowbrick.__version__)
/usr/local/lib/python3.7/dist-packages/statsmodels/tools/_testing.py:19: FutureWarning: pandas.util.testing is deprecated. Use the functions in the public API at pandas.testing instead.
    import pandas.util.testing as tm
2.7.0
0.9.1

```

In [2]:

```

from google.colab import drive
drive.mount('/content/drive')
Mounted at /content/drive

```

In [3]:

```

os.getcwd()
df = pd.read_csv('./drive/MyDrive/data/all_train.csv')
df.shape
df.head()

```

Out[3]:

```

'/content'

```

Out[3]:

```

(7000000, 29)

```

Out[3]:

In []:

```

df['# label'].value_counts()

```

Out[]:

```

1.0      3500879
0.0      3499121
Name: # label, dtype: int64

```

In []:

```

#Check class distribution
%matplotlib inline

# Adapted from:
# https://www.featureranking.com/tutorials/machine-learning-tutorials/information-gain-computation/
def gini_index(y):
    probs = pd.value_counts(y, normalize=True)

```

```

    return 1 - np.sum(np.square(probs))

def plot_class_dist(y):
    class_ct = len(np.unique(y['# label']))
    vc = pd.value_counts(y['# label'])
    print('Total Records', len(y['# label']))
    print('Total Classes:', class_ct)
    print('Smallest Class Id:',vc.idxmin(),'Records:',vc.min())
    print('Largest Class Id:',vc.idxmax(),'Records:',vc.max())

    position_counts = pd.DataFrame(y['# label'].value_counts())
    position_counts['Percentage'] = position_counts['# label']/position_counts.sum()[0]
    print(position_counts)
    plt.figure(figsize=(4,4))
    plt.pie(position_counts['Percentage'],labels = ['yes', 'no']);

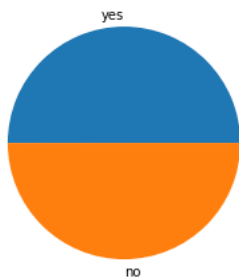
```

```

plot_class_dist(df.iloc[:,0:1])
Total Records 7000000
Total Classes: 2
Smallest Class Id: 0.0 Records: 3499121
Largest Class Id: 1.0 Records: 3500879

```

	# label	Percentage
1.0	3500879	0.500126
0.0	3499121	0.499874



In []:

```
df.describe().T
```

Out[]:

	count	mean	std	min	25%	50%	75%	max
# label	7000000	0.500126	0.500000	0.000000	0.000000	1.000000	1.000000	1.000000

f0	7000000. 0	0.016125	1.004417	-1.960549	-0.728821	-0.039303	0.690080	4.378282
f1	7000000. 0	0.000477	0.997486	-2.365355	-0.733255	0.000852	0.734783	2.365287
f2	7000000. 0	0.000027	1.000080	-1.732165	-0.865670	0.000320	0.865946	1.732370
f3	7000000. 0	0.010561	0.995600	-9.980274	-0.609229	0.019633	0.679882	4.148023
f4	7000000. 0	-0.000105	0.999867	-1.732137	-0.865802	-0.000507	0.865765	1.731978
f5	7000000. 0	0.002766	1.000957	-1.054221	-1.054221	-0.005984	0.850488	4.482618
f6	7000000. 0	0.018160	0.986775	-3.034787	-0.756609	-0.149953	0.768669	3.720345
f7	7000000. 0	0.000025	0.996587	-2.757853	-0.701415	-0.000107	0.701319	2.758590
f8	7000000. 0	0.000435	1.000007	-1.732359	-0.865654	0.001385	0.866598	1.731450
f9	7000000. 0	-0.006870	1.001938	-1.325801	-1.325801	0.754261	0.754261	0.754261
f10	7000000. 0	0.017543	0.994151	-2.835563	-0.723727	-0.128573	0.647864	4.639335
f11	7000000. 0	-0.000161	0.998450	-2.602091	-0.703293	-0.000576	0.704100	2.602294
f12	7000000. 0	-0.000329	1.000078	-1.732216	-0.866599	-0.001282	0.865832	1.732007
f13	7000000. 0	0.001739	0.999737	-1.161915	-1.161915	0.860649	0.860649	0.860649

f14	7000000. 0	0.017246	0.999465	-2.454879	-0.699618	-0.097493	0.634705	5.535799
f15	7000000. 0	0.000483	0.998429	-2.437812	-0.707026	0.000298	0.708371	2.438369
f16	7000000. 0	-0.000554	0.999861	-1.732145	-0.866247	-0.001377	0.864942	1.732738
f17	7000000. 0	0.004960	1.001006	-0.815440	-0.815440	-0.815440	1.226331	1.226331
f18	7000000. 0	0.011648	1.002725	-1.728284	-0.742363	-0.089925	0.642319	5.866367
f19	7000000. 0	-0.000113	1.000038	-2.281867	-0.720685	-0.000067	0.720492	2.282217
f20	7000000. 0	0.000077	1.000033	-1.731758	-0.865685	-0.000442	0.865957	1.732740
f21	7000000. 0	0.000291	1.000170	-0.573682	-0.573682	-0.573682	-0.573682	1.743123
f22	7000000. 0	0.012288	1.010477	-3.631608	-0.541794	-0.160276	0.481219	7.293420
f23	7000000. 0	0.009778	1.005418	-4.729473	-0.511552	-0.314403	0.163489	9.333287
f24	7000000. 0	0.005270	1.009990	-20.622229	-0.354387	-0.326523	-0.233767	14.990636
f25	7000000. 0	-0.001761	0.984451	-3.452634	-0.692510	-0.357030	0.475313	5.277313
f26	7000000. 0	0.015331	0.982280	-2.632761	-0.794380	-0.088286	0.761085	4.444690
mas s	7000000. 0	1000.10738 7	353.42548 7	499.99996 9	750.00000 0	1000.00000 0	1250.00000 0	1500.00000 0

In []:

```

def print_highly_correlated(df, features, t=0.8):
    #Method will extract out features that are correlated based on thresh hold
    l = []
    c_df = df[features].corr() # get correlations
    cor_features = np.where(np.abs(c_df) > t) # nparray method
    cor_features = [(c_df.iloc[x,y], x, y) for x, y in zip(*cor_features) if
x != y and x < y]
    #try sorting
    corr_list = sorted(cor_features, key=lambda x: -abs(x[0]))
    if corr_list == []:
        print("Nothing above: ", t)
    else:

        for v, i, j in corr_list:
            cols = df[features].columns
            if c_df.index[i] not in l:
                l.append(c_df.index[i])
            if c_df.index[j] not in l:
                l.append(c_df.index[j])
            print ("%s and %s = %.3f" % (c_df.index[i], c_df.columns[j], v))
    return l

```

```
print_highly_correlated(df, df.columns, t=0.96)
```

```

#prepare the plot pallete
#cmap = sns.diverging_palette(220, 10, as_cmap=True) # one of the many color
mappings
#sns.set(style="darkgrid") # one of the many styles to plot using
#f, ax = plt.subplots(figsize=(25, 25))
#%time sns.heatmap(df_imputed[print_highly_correlated(df, df.columns, t=0.99
)].corr(), cmap=cmap, fmt=".2f",annot=True);
#f.tight_layout();
Nothing above: 0.96

```

Out[]:

```
[]
```

In []:

```

percent_missing = df.isnull().sum() * 100 / len(df)
missing_value_df = pd.DataFrame({'column_name': df.columns,
                                'percent_missing': percent_missing})
missing_value_df.sort_values('percent_missing', inplace=True, ascending=False)
missing_value_df.head(15)

```

Out[]:

	column_name	percent_missing
# label	# label	0.0
f14	f14	0.0
f26	f26	0.0
f25	f25	0.0
f24	f24	0.0
f23	f23	0.0
f22	f22	0.0
f21	f21	0.0
f20	f20	0.0
f19	f19	0.0
f18	f18	0.0
f17	f17	0.0
f16	f16	0.0
f15	f15	0.0
f13	f13	0.0

In [4]:

```
X = df.iloc[:,1:].values
X.shape
y = df['# label'].values
y.shape
```

```

#Normalize data
##Scale the transformed data ### for relu 0, 1
scl_obj = MinMaxScaler(feature_range=[0, 1]) #StandardScaler()
scl_obj.fit(X)
X_scaled = scl_obj.transform(X)
#QuantileTransformer(output_distribution='uniform').fit_transform(X)
X_scaled.shape

```

```

#X_scaled

```

Out[4]:

```

(7000000, 28)

```

Out[4]:

```

(7000000,)

```

Out[4]:

```

MinMaxScaler(copy=True, feature_range=[0, 1])

```

Out[4]:

```

(7000000, 28)

```

In []:

```

scaled_train_df = pd.DataFrame(X_scaled, columns=df.iloc[:,1:].columns.values)

```

```

for i in scaled_train_df:
    scaled_train_df[i].hist()
    plt.show()

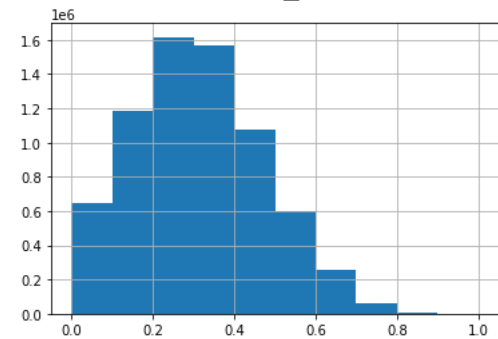
```

Out[]:

```

<matplotlib.axes._subplots.AxesSubplot at 0x7f8265673610>

```

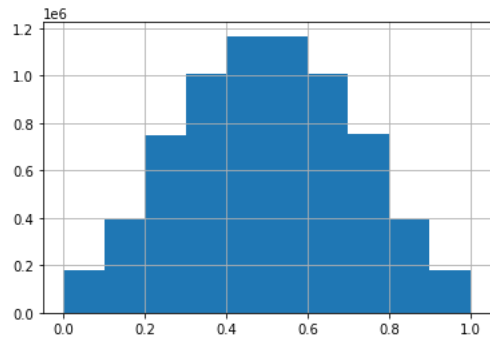


Out[]:

```

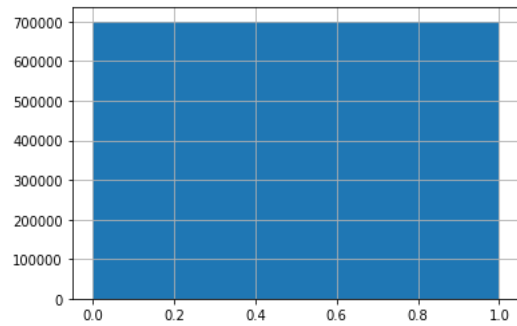
<matplotlib.axes._subplots.AxesSubplot at 0x7f82655f3350>

```



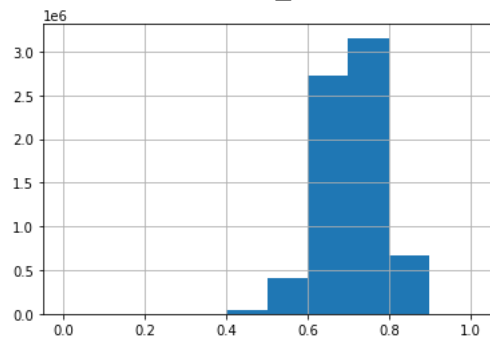
Out[]:

<matplotlib.axes._subplots.AxesSubplot at 0x7f8265547dd0>



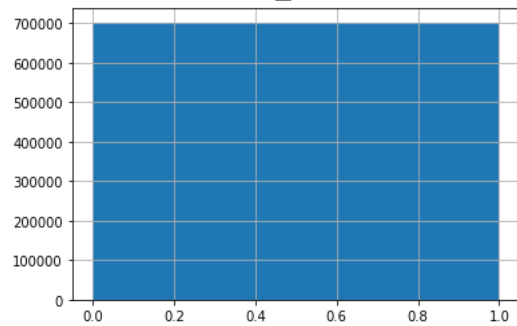
Out[]:

<matplotlib.axes._subplots.AxesSubplot at 0x7f82655291d0>



Out[]:

<matplotlib.axes._subplots.AxesSubplot at 0x7f82654a0cd0>

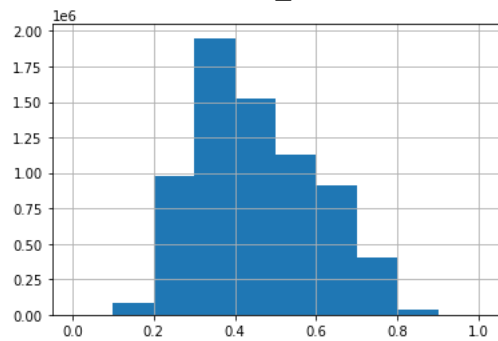


Out[]:

<matplotlib.axes._subplots.AxesSubplot at 0x7f82654a0590>

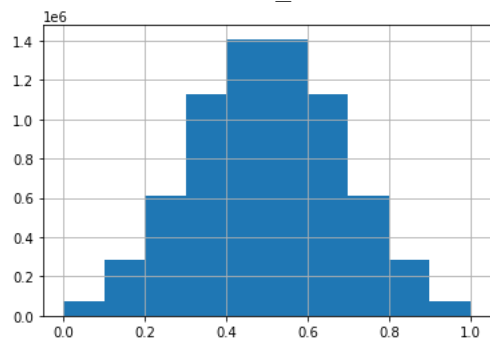
Out[]:

<matplotlib.axes._subplots.AxesSubplot at 0x7f8265342b50>



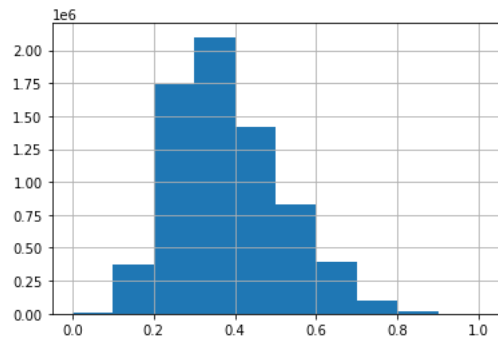
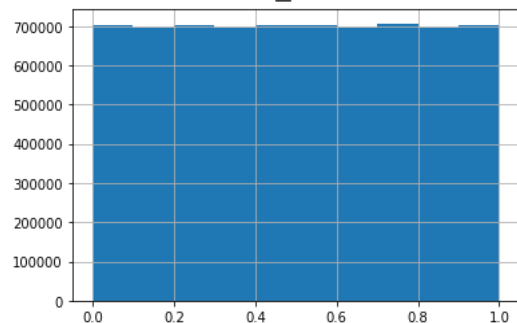
Out[]:

<matplotlib.axes._subplots.AxesSubplot at 0x7f826527b490>



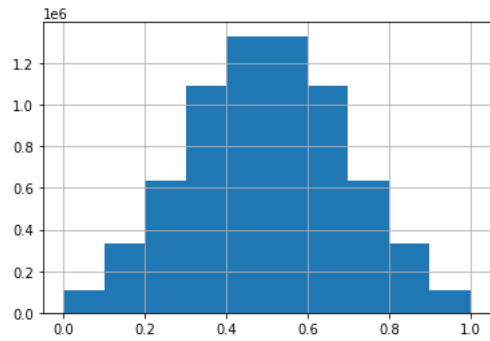
Out[]:

<matplotlib.axes._subplots.AxesSubplot at 0x7f82652677d0>



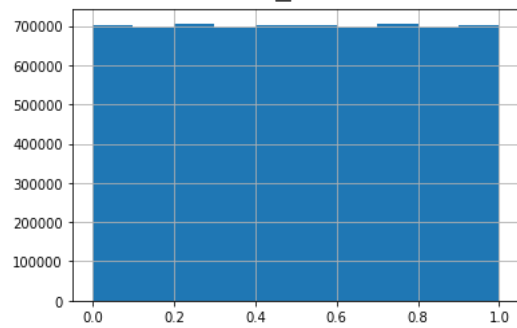
Out[]:

<matplotlib.axes._subplots.AxesSubplot at 0x7f826509b110>

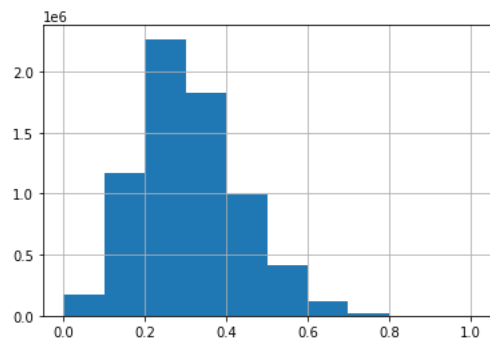


Out[]:

<matplotlib.axes._subplots.AxesSubplot at 0x7f82651223d0>

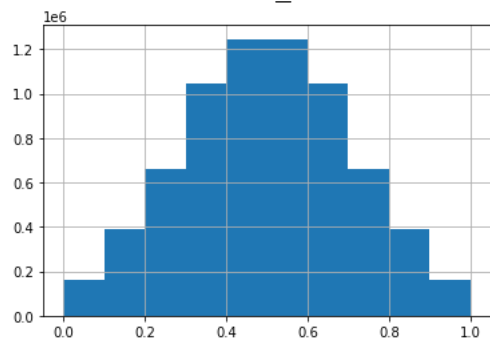


Out[]:

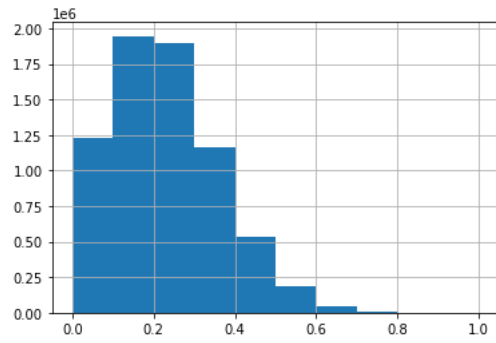


Out[]:

<matplotlib.axes._subplots.AxesSubplot at 0x7f8264e5d410>

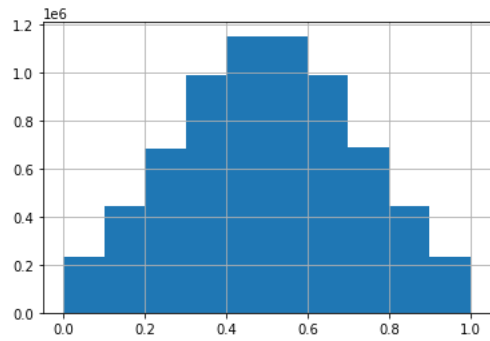


Out[]:



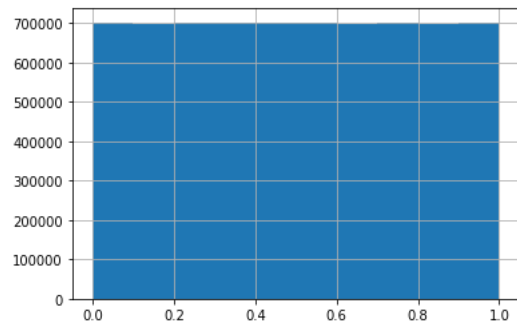
Out[]:

<matplotlib.axes._subplots.AxesSubplot at 0x7f82651a4910>

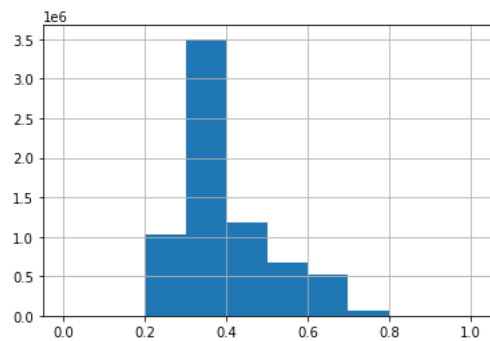


Out[]:

<matplotlib.axes._subplots.AxesSubplot at 0x7f8265509d50>

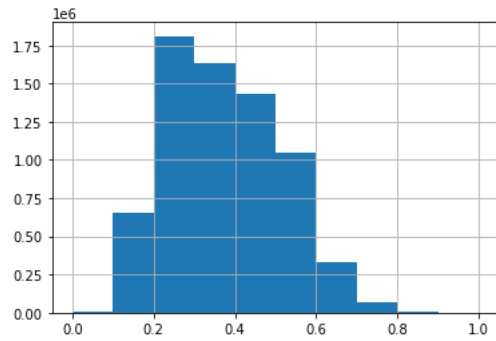


Out[]:



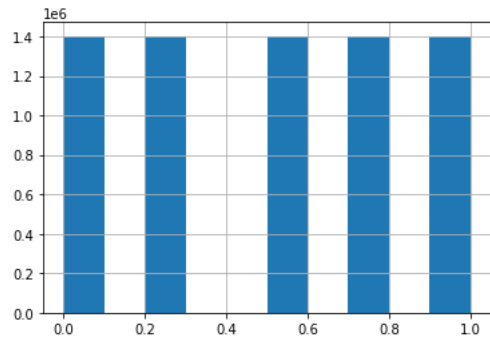
Out[]:

<matplotlib.axes._subplots.AxesSubplot at 0x7f82652cf610>



Out[]:

<matplotlib.axes._subplots.AxesSubplot at 0x7f826503c090>



In [5]:

```
#modeltrain/hold 90/10 stratified
stt = StratifiedShuffleSplit(n_splits=1, test_size=0.1, random_state=45)
train_index_clf, test_index_clf = next(stt.split(X_scaled, y))
X_trainmodel = X[train_index_clf]
y_trainmodel = y[train_index_clf].ravel()
X_hold = X[test_index_clf]
y_hold = y[test_index_clf].ravel()
X_trainmodel.shape
y_trainmodel.shape
X_hold.shape
y_hold.shape
```

Out[5]:

(6300000, 28)

Out[5]:

(6300000,)

Out[5]:

(700000, 28)

Out[5]:

(700000,)

In [6]:

```
#train/test 80/20 stratified
stt = StratifiedShuffleSplit(n_splits=1, test_size=0.2, random_state=45)
```

```

train_index_clf, test_index_clf = next(stt.split(X_trainmodel, y_trainmodel)
)
X_train = X[train_index_clf]
y_train = y[train_index_clf].ravel()
X_test = X[test_index_clf]
y_test = y[test_index_clf].ravel()

```

```

X_train.shape
y_train.shape
X_test.shape
y_test.shape

```

Out [6]:

```
(5040000, 28)
```

Out [6]:

```
(5040000,)
```

Out [6]:

```
(1260000, 28)
```

Out [6]:

```
(1260000,)
```

In [7]:

```

def FindLayerNodesLinear(n_layers, first_layer_nodes, last_layer_nodes):
    layers = []

    nodes_increment = (last_layer_nodes - first_layer_nodes) / (n_layers-1)
    nodes = first_layer_nodes
    for i in range(1, n_layers+1):
        layers.append(math.ceil(nodes))
        nodes = nodes + nodes_increment

    return layers

```

In [8]:

```

from tensorflow.keras.callbacks import EarlyStopping
model_clf_stats = pd.DataFrame()

def createmodel(n_layers, first_layer_nodes, last_layer_nodes, activation_func, loss_func):
    model = Sequential()
    n_nodes = FindLayerNodesLinear(n_layers, first_layer_nodes, last_layer_nodes)
    for i in range(1, n_layers):

        if i==1:
            print("building node:", i)

```

```

        model.add(Dense(first_layer_nodes, input_dim=X_train.shape[1], activation=activation_func))
    else:
        print("building node:", i)
        model.add(Dense(n_nodes[i-1], activation=activation_func))

    #Finally, the output layer should have a single node in binary classification
    model.add(Dense(1, activation='sigmoid'))
    model.compile(optimizer='adam', loss=loss_func, metrics = ["accuracy"])
    #note: metrics could also be 'mse'

    return model

```

In [9]:

```

def test_model(layers, start, end, activation, batch, X_train, y_train, X_test, y_test, ver=1):
    #relu, l=5, nodes=600, e_nodes=8, e=500, b=20000
    print("*****Execution started for*****")
    print("Activation:", activation, " layers:", layers, " nodes:", start, " batch:", batch)
    safety = EarlyStopping(monitor='val_loss', patience=5)
    seed = 45 #88.27
    m = createmodel(n_layers=layers, first_layer_nodes=start, last_layer_nodes=end,
                    activation_func=activation, loss_func=tf.keras.losses.BinaryCrossentropy()) #tanh
    hist = m.fit(X_train, y_train, epochs=500, batch_size=batch,
                validation_data=(X_test, y_test), callbacks=[safety], verbose=ver)
    # add validation left out here

    best_score = max(hist.history['accuracy'])
    print("Best score: ", best_score)
    model_stat = pd.DataFrame()
    model_stat['Accuracy'] = [best_score]
    model_stat['Model'] = ["Activation:" + activation + " layers:" + str(layers) + " nodes:" + str(start) + " batch:" + str(batch)]
    m.summary()
    tf.keras.backend.clear_session()
    del m
    print("*****Execution ended*****")
    print("*****\n\n")
    return model_stat

```

In [63]:

```
#p, m = test_model(3, 400, 8, 'relu', 10000, X_train, y_train, X_test, y_test)
#tf.keras.backend.clear_session()
#del m
```

In [66]:

```
p = test_model(3, 400, 8, 'relu', 10000, X_train, y_train, X_test, y_test)
model_clf_stats = model_clf_stats.append(p)
```

```
p = test_model(3, 600, 8, 'relu', 10000, X_train, y_train, X_test, y_test)
model_clf_stats = model_clf_stats.append(p)
```

```
p = test_model(3, 800, 8, 'relu', 10000, X_train, y_train, X_test, y_test)
model_clf_stats = model_clf_stats.append(p)
```

```
model_clf_stats
```

```
*****Execution started for*****
```

```
Activation: relu layers: 3 nodes: 400 batch: 10000
```

```
building node: 1
```

```
building node: 2
```

```
Epoch 1/500
```

```
504/504 [=====] - 3s 5ms/step - loss: 1.2628 - accuracy: 0.7409 - val_loss: 0.4395 - val_accuracy: 0.7955
```

```
Epoch 2/500
```

```
504/504 [=====] - 2s 4ms/step - loss: 0.5452 - accuracy: 0.7825 - val_loss: 5.9589 - val_accuracy: 0.4992
```

```
Epoch 3/500
```

```
...
```

```
Epoch 70/500
```

```
504/504 [=====] - 2s 4ms/step - loss: 0.2698 - accuracy: 0.8782 - val_loss: 0.2707 - val_accuracy: 0.8777
```

```
Best score: 0.8781597018241882
```

```
Model: "sequential_2"
```

Layer (type)	Output Shape	Param #
dense_6 (Dense)	(None, 400)	11600
dense_7 (Dense)	(None, 204)	81804
dense_8 (Dense)	(None, 1)	205

```
=====  
Total params: 93,609
```

```
Trainable params: 93,609
```

Non-trainable params: 0

*****Execution ended*****

*****Execution started for*****

Activation: relu layers: 3 nodes: 600 batch: 10000

building node: 1

building node: 2

Epoch 1/500

504/504 [=====] - 3s 6ms/step - loss: 1.4198 - accuracy: 0.7220 - val_loss: 1.6064 - val_accuracy: 0.5557

...

504/504 [=====] - 3s 6ms/step - loss: 0.2640 - accuracy: 0.8814 - val_loss: 0.2662 - val_accuracy: 0.8802

Best score: 0.8813777565956116

Model: "sequential"

Layer (type)	Output Shape	Param #
=====		
dense (Dense)	(None, 600)	17400
dense_1 (Dense)	(None, 304)	182704
dense_2 (Dense)	(None, 1)	305

Total params: 200,409

Trainable params: 200,409

Non-trainable params: 0

*****Execution ended*****

*****Execution started for*****

Activation: relu layers: 3 nodes: 800 batch: 10000

building node: 1

building node: 2

Epoch 1/500

504/504 [=====] - 4s 7ms/step - loss: 2.3333 - accuracy: 0.7142 - val_loss: 0.4521 - val_accuracy: 0.8181

Epoch 2/500

```

504/504 [=====] - 3s 7ms/step - loss: 0.6233 - accuracy: 0.7695 - val_loss: 0.3900 - val_accuracy: 0.8263
...
504/504 [=====] - 4s 7ms/step - loss: 0.2600 - accuracy: 0.8836 - val_loss: 0.2630 - val_accuracy: 0.8819
Best score: 0.8836385011672974
Model: "sequential"

```

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 800)	23200
dense_1 (Dense)	(None, 404)	323604
dense_2 (Dense)	(None, 1)	405

```

=====
Total params: 347,209
Trainable params: 347,209
Non-trainable params: 0

```

```

*****Execution ended*****
*****

```

Out[66]:

	Accuracy	Model
0	0.878160	Activation:relu layers:3 nodes:400 batch:10000
0	0.881378	Activation:relu layers:3 nodes:600 batch:10000
0	0.883639	Activation:relu layers:3 nodes:800 batch:10000

In [67]:

```

p = test_model(3, 400, 8, 'relu', 20000, X_train, y_train, X_test, y_test)
model_clf_stats = model_clf_stats.append(p)

p = test_model(3, 600, 8, 'relu', 20000, X_train, y_train, X_test, y_test)
model_clf_stats = model_clf_stats.append(p)

p = test_model(3, 800, 8, 'relu', 20000, X_train, y_train, X_test, y_test)
model_clf_stats = model_clf_stats.append(p)

```

```

model_clf_stats
*****Execution started for*****
Activation: relu  layers: 3  nodes: 400  batch: 20000
building node: 1
building node: 2
Epoch 1/500
252/252 [=====] - 2s 7ms/step - loss: 1.9611 - accu
racy: 0.6956 - val_loss: 0.4396 - val_accuracy: 0.8073
...
252/252 [=====] - 1s 6ms/step - loss: 0.3127 - accu
racy: 0.8561 - val_loss: 0.3115 - val_accuracy: 0.8579
Epoch 45/500
252/252 [=====] - 1s 6ms/step - loss: 0.3187 - accu
racy: 0.8530 - val_loss: 0.3098 - val_accuracy: 0.8578
Best score:  0.8561081290245056
Model: "sequential"

```

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 400)	11600
dense_1 (Dense)	(None, 204)	81804
dense_2 (Dense)	(None, 1)	205

```

=====
Total params: 93,609
Trainable params: 93,609
Non-trainable params: 0

```

```

*****Execution ended*****
*****

```

```

*****Execution started for*****
Activation: relu  layers: 3  nodes: 600  batch: 20000
building node: 1
building node: 2
Epoch 1/500
252/252 [=====] - 3s 10ms/step - loss: 3.6500 - acc
uracy: 0.6804 - val_loss: 0.4217 - val_accuracy: 0.8168
Epoch 2/500

```



```

252/252 [=====] - 2s 9ms/step - loss: 0.5889 - accu
racy: 0.7594 - val_loss: 0.4149 - val_accuracy: 0.8231
...
252/252 [=====] - 2s 9ms/step - loss: 0.3760 - accu
racy: 0.8283 - val_loss: 0.3551 - val_accuracy: 0.8303
Epoch 16/500
252/252 [=====] - 2s 9ms/step - loss: 0.3759 - accu
racy: 0.8277 - val_loss: 0.4047 - val_accuracy: 0.8053
Epoch 17/500
252/252 [=====] - 2s 9ms/step - loss: 0.4296 - accu
racy: 0.8141 - val_loss: 0.3726 - val_accuracy: 0.8240
Epoch 18/500
252/252 [=====] - 2s 9ms/step - loss: 0.4188 - accu
racy: 0.8191 - val_loss: 0.3583 - val_accuracy: 0.8378
Best score: 0.8362652659416199
Model: "sequential"

```

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 600)	17400
dense_1 (Dense)	(None, 304)	182704
dense_2 (Dense)	(None, 1)	305

```

=====
Total params: 200,409
Trainable params: 200,409
Non-trainable params: 0

```

```

*****Execution ended*****
*****

```

```

*****Execution started for*****
Activation: relu layers: 3 nodes: 800 batch: 20000
building node: 1
building node: 2
Epoch 1/500
252/252 [=====] - 4s 13ms/step - loss: 4.3767 - acc
uracy: 0.6665 - val_loss: 0.4411 - val_accuracy: 0.8118
...
252/252 [=====] - 3s 12ms/step - loss: 0.3140 - acc
uracy: 0.8546 - val_loss: 0.3127 - val_accuracy: 0.8542

```

```
Epoch 34/500
252/252 [=====] - 3s 12ms/step - loss: 0.3125 - acc
uracy: 0.8551 - val_loss: 0.3198 - val_accuracy: 0.8554
Best score: 0.855080783367157
Model: "sequential"
```

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 800)	23200
dense_1 (Dense)	(None, 404)	323604
dense_2 (Dense)	(None, 1)	405

```
=====  
Total params: 347,209  
Trainable params: 347,209  
Non-trainable params: 0
```

```
*****Execution ended*****  
*****
```

Out[67]:

Accuracy		Model
0	0.878160	Activation:relu layers:3 nodes:400 batch:10000
0	0.881378	Activation:relu layers:3 nodes:600 batch:10000
0	0.883639	Activation:relu layers:3 nodes:800 batch:10000
0	0.856108	Activation:relu layers:3 nodes:400 batch:20000
0	0.836265	Activation:relu layers:3 nodes:600 batch:20000
0	0.855081	Activation:relu layers:3 nodes:800 batch:20000

In [68]:

```
p = test_model(5, 400, 8, 'relu', 10000, X_train, y_train, X_test, y_test)
model_clf_stats = model_clf_stats.append(p)
```

```

p = test_model(5, 600, 8, 'relu', 10000, X_train, y_train, X_test, y_test)
model_clf_stats = model_clf_stats.append(p)

p = test_model(5, 800, 8, 'relu', 10000, X_train, y_train, X_test, y_test)
model_clf_stats = model_clf_stats.append(p)

model_clf_stats
*****Execution started for*****
Activation: relu  layers: 5  nodes: 400  batch: 10000
building node: 1
building node: 2
building node: 3
building node: 4
Epoch 1/500
504/504 [=====] - 4s 7ms/step - loss: 0.8635 - accu
racy: 0.7412 - val_loss: 0.3898 - val_accuracy: 0.8235
Epoch 2/500
504/504 [=====] - 3s 6ms/step - loss: 0.3927 - accu
racy: 0.8176 - val_loss: 0.3812 - val_accuracy: 0.8197
...
504/504 [=====] - 3s 6ms/step - loss: 0.2633 - accu
racy: 0.8816 - val_loss: 0.2649 - val_accuracy: 0.8807
Epoch 48/500
504/504 [=====] - 3s 6ms/step - loss: 0.2634 - accu
racy: 0.8815 - val_loss: 0.2647 - val_accuracy: 0.8806
Epoch 49/500
504/504 [=====] - 3s 6ms/step - loss: 0.2632 - accu
racy: 0.8818 - val_loss: 0.2652 - val_accuracy: 0.8804
Best score:  0.8817861080169678
Model: "sequential"

```

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 400)	11600
dense_1 (Dense)	(None, 302)	121102
dense_2 (Dense)	(None, 204)	61812
dense_3 (Dense)	(None, 106)	21730
dense_4 (Dense)	(None, 1)	107

```
=====
Total params: 216,351
Trainable params: 216,351
Non-trainable params: 0

```

```
*****Execution ended*****
*****

```

```
*****Execution started for*****

```

```
Activation: relu layers: 5 nodes: 600 batch: 10000

```

```
building node: 1

```

```
building node: 2

```

```
building node: 3

```

```
building node: 4

```

```
Epoch 1/500

```

```
504/504 [=====] - 6s 10ms/step - loss: 0.8281 - accu
racy: 0.7444 - val_loss: 0.3882 - val_accuracy: 0.8230

```

```
Epoch 2/500

```

```
504/504 [=====] - 5s 9ms/step - loss: 0.4050 - accu
racy: 0.8108 - val_loss: 0.3587 - val_accuracy: 0.8306

```

```
...

```

```
504/504 [=====] - 5s 9ms/step - loss: 0.2592 - accu
racy: 0.8839 - val_loss: 0.2629 - val_accuracy: 0.8817

```

```
Epoch 65/500

```

```
504/504 [=====] - 5s 9ms/step - loss: 0.2588 - accu
racy: 0.8840 - val_loss: 0.2636 - val_accuracy: 0.8814

```

```
Epoch 66/500

```

```
504/504 [=====] - 5s 9ms/step - loss: 0.2590 - accu
racy: 0.8840 - val_loss: 0.2627 - val_accuracy: 0.8821

```

```
Best score: 0.8840420842170715

```

```
Model: "sequential"

```

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 600)	17400
dense_1 (Dense)	(None, 452)	271652
dense_2 (Dense)	(None, 304)	137712
dense_3 (Dense)	(None, 156)	47580
dense_4 (Dense)	(None, 1)	157

```

=====
Total params: 474,501
Trainable params: 474,501
Non-trainable params: 0

*****Execution ended*****
*****

*****Execution started for*****
Activation: relu layers: 5 nodes: 800 batch: 10000
building node: 1
building node: 2
building node: 3
building node: 4
Epoch 1/500
504/504 [=====] - 7s 14ms/step - loss: 1.1224 - acc
uracy: 0.7436 - val_loss: 0.3881 - val_accuracy: 0.8219
...
Epoch 59/500
504/504 [=====] - 7s 13ms/step - loss: 0.2575 - acc
uracy: 0.8848 - val_loss: 0.2634 - val_accuracy: 0.8820
Epoch 60/500
504/504 [=====] - 7s 13ms/step - loss: 0.2574 - acc
uracy: 0.8850 - val_loss: 0.2615 - val_accuracy: 0.8824
Epoch 61/500
504/504 [=====] - 7s 13ms/step - loss: 0.2572 - acc
uracy: 0.8850 - val_loss: 0.2618 - val_accuracy: 0.8827
Best score: 0.8850095272064209
Model: "sequential"

```

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 800)	23200
dense_1 (Dense)	(None, 602)	482202
dense_2 (Dense)	(None, 404)	243612
dense_3 (Dense)	(None, 206)	83430
dense_4 (Dense)	(None, 1)	207

```
=====
Total params: 832,651
Trainable params: 832,651
Non-trainable params: 0
```

```
*****Execution ended*****
*****
```

Out[68]:

	Accuracy	Model
0	0.878160	Activation:relu layers:3 nodes:400 batch:10000
0	0.881378	Activation:relu layers:3 nodes:600 batch:10000
0	0.883639	Activation:relu layers:3 nodes:800 batch:10000
0	0.856108	Activation:relu layers:3 nodes:400 batch:20000
0	0.836265	Activation:relu layers:3 nodes:600 batch:20000
0	0.855081	Activation:relu layers:3 nodes:800 batch:20000
0	0.881786	Activation:relu layers:5 nodes:400 batch:10000
0	0.884042	Activation:relu layers:5 nodes:600 batch:10000
0	0.885010	Activation:relu layers:5 nodes:800 batch:10000

In [69]:

```
p = test_model(5, 400, 8, 'relu', 20000, X_train, y_train, X_test, y_test)
model_clf_stats = model_clf_stats.append(p)

p = test_model(5, 600, 8, 'relu', 20000, X_train, y_train, X_test, y_test)
model_clf_stats = model_clf_stats.append(p)

p = test_model(5, 800, 8, 'relu', 20000, X_train, y_train, X_test, y_test)
model_clf_stats = model_clf_stats.append(p)
```

```

model_clf_stats
*****Execution started for*****
Activation: relu  layers: 5  nodes: 400  batch: 20000
building node: 1
building node: 2
building node: 3
building node: 4
Epoch 1/500
252/252 [=====] - 3s 11ms/step - loss: 1.3383 - acc
uracy: 0.7007 - val_loss: 0.4294 - val_accuracy: 0.8067
...
252/252 [=====] - 3s 11ms/step - loss: 0.2647 - acc
uracy: 0.8809 - val_loss: 0.2668 - val_accuracy: 0.8797
Epoch 88/500
252/252 [=====] - 3s 11ms/step - loss: 0.2644 - acc
uracy: 0.8811 - val_loss: 0.2656 - val_accuracy: 0.8803
Epoch 89/500
252/252 [=====] - 3s 11ms/step - loss: 0.2645 - acc
uracy: 0.8810 - val_loss: 0.2657 - val_accuracy: 0.8802
Best score:  0.8810511827468872
Model: "sequential"

```

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 400)	11600
dense_1 (Dense)	(None, 302)	121102
dense_2 (Dense)	(None, 204)	61812
dense_3 (Dense)	(None, 106)	21730
dense_4 (Dense)	(None, 1)	107

```

=====
Total params: 216,351
Trainable params: 216,351
Non-trainable params: 0

```

```

*****Execution ended*****
*****

```

```

*****Execution started for*****

```

```

Activation: relu  layers: 5  nodes: 600  batch: 20000
building node: 1
building node: 2
building node: 3
building node: 4
Epoch 1/500
252/252 [=====] - 5s 17ms/step - loss: 1.8562 - acc
uracy: 0.6664 - val_loss: 0.4256 - val_accuracy: 0.8077
...
252/252 [=====] - 4s 16ms/step - loss: 0.2624 - acc
uracy: 0.8820 - val_loss: 0.2646 - val_accuracy: 0.8807
Epoch 89/500
252/252 [=====] - 4s 16ms/step - loss: 0.2619 - acc
uracy: 0.8823 - val_loss: 0.2640 - val_accuracy: 0.8811
Best score:  0.8822767734527588
Model: "sequential"

```

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 600)	17400
dense_1 (Dense)	(None, 452)	271652
dense_2 (Dense)	(None, 304)	137712
dense_3 (Dense)	(None, 156)	47580
dense_4 (Dense)	(None, 1)	157

```

=====
Total params: 474,501
Trainable params: 474,501
Non-trainable params: 0

```

```

*****Execution ended*****
*****

```

```

*****Execution started for*****
Activation: relu  layers: 5  nodes: 800  batch: 20000
building node: 1
building node: 2
building node: 3
building node: 4

```



```
Epoch 1/500
252/252 [=====] - 7s 25ms/step - loss: 1.9167 - acc
uracy: 0.6863 - val_loss: 0.4180 - val_accuracy: 0.8077
Epoch 2/500
252/252 [=====] - 6s 24ms/step - loss: 0.4175 - acc
uracy: 0.8018 - val_loss: 0.3867 - val_accuracy: 0.8188
...
252/252 [=====] - 6s 24ms/step - loss: 0.2791 - acc
uracy: 0.8726 - val_loss: 0.2782 - val_accuracy: 0.8732
Epoch 50/500
252/252 [=====] - 6s 24ms/step - loss: 0.2768 - acc
uracy: 0.8740 - val_loss: 0.2764 - val_accuracy: 0.8740
Best score: 0.877587080001831
Model: "sequential"
```

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 800)	23200
dense_1 (Dense)	(None, 602)	482202
dense_2 (Dense)	(None, 404)	243612
dense_3 (Dense)	(None, 206)	83430
dense_4 (Dense)	(None, 1)	207

```
=====
Total params: 832,651
Trainable params: 832,651
Non-trainable params: 0
```

```
*****Execution ended*****
*****
```

Out[69]:

	Accuracy	Model
0	0.878160	Activation:relu layers:3 nodes:400 batch:10000
0	0.881378	Activation:relu layers:3 nodes:600 batch:10000

0 0.883639 Activation:relu layers:3 nodes:800 batch:10000

0 0.856108 Activation:relu layers:3 nodes:400 batch:20000

0 0.836265 Activation:relu layers:3 nodes:600 batch:20000

0 0.855081 Activation:relu layers:3 nodes:800 batch:20000

0 0.881786 Activation:relu layers:5 nodes:400 batch:10000

0 0.884042 Activation:relu layers:5 nodes:600 batch:10000

0 0.885010 Activation:relu layers:5 nodes:800 batch:10000

0 0.881051 Activation:relu layers:5 nodes:400 batch:20000

0 0.882277 Activation:relu layers:5 nodes:600 batch:20000

0 0.877587 Activation:relu layers:5 nodes:800 batch:20000

In [10]:

```
#Refit best model to get reference
```

```
safety = EarlyStopping(monitor='val_loss', patience=5)
```

```
seed = 45 #88.27
```

```
m = createmodel(n_layers=5, first_layer_nodes=600, last_layer_nodes=8,  
                activation_func='relu', loss_func=tf.keras.losses.BinaryCrossentropy()) #tanh
```

```
hist = m.fit(X_train, y_train, epochs=500, batch_size=10000,  
            validation_data=(X_test, y_test), callbacks=[safety], verbose=1) # add validation left out here
```

```
best_score = max(hist.history['accuracy'])
```

```
print("Best score: ",best_score)
```

```
building node: 1
```

```
building node: 2
```

```
building node: 3
```

```
building node: 4
```

```
Epoch 1/500
```

```

504/504 [=====] - 7s 10ms/step - loss: 0.9710 - acc
uracy: 0.7246 - val_loss: 0.3895 - val_accuracy: 0.8203
Epoch 2/500
504/504 [=====] - 5s 9ms/step - loss: 0.3894 - accu
racy: 0.8184 - val_loss: 0.3650 - val_accuracy: 0.8266
...
504/504 [=====] - 5s 9ms/step - loss: 0.2604 - accu
racy: 0.8832 - val_loss: 0.2620 - val_accuracy: 0.8823
Epoch 54/500
504/504 [=====] - 5s 9ms/step - loss: 0.2600 - accu
racy: 0.8834 - val_loss: 0.2623 - val_accuracy: 0.8822
Best score: 0.8834400773048401

```

In [14]:

```

m.summary()
Model: "sequential"

```

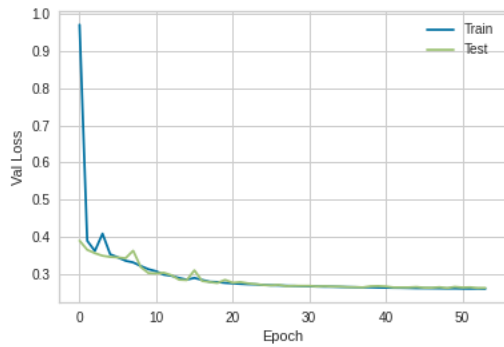
Layer (type)	Output Shape	Param #
dense (Dense)	(None, 600)	17400
dense_1 (Dense)	(None, 452)	271652
dense_2 (Dense)	(None, 304)	137712
dense_3 (Dense)	(None, 156)	47580
dense_4 (Dense)	(None, 1)	157
Total params: 474,501		
Trainable params: 474,501		
Non-trainable params: 0		

In [15]:

```

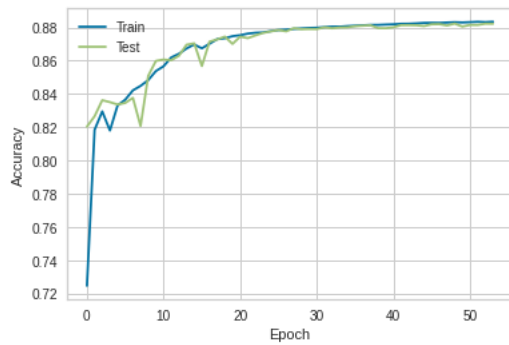
train_loss = m.history.history['loss']
val_loss = m.history.history['val_loss']
_=plt.plot(train_loss, label='Train')
_=plt.plot(val_loss, label='Test')
_=plt.xlabel("Epoch")
_=plt.ylabel("Val Loss")
_=plt.legend()
plt.show()

```



In [14]:

```
train_acc = m.history.history['accuracy']
val_acc = m.history.history['val_accuracy']
_=plt.plot(train_acc, label='Train')
_=plt.plot(val_acc, label='Test')
_=plt.xlabel("Epoch")
_=plt.ylabel("Accuracy")
_=plt.legend()
plt.show()
```



In [49]:

```
m.summary()
Model: "sequential"
```

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 400)	11600
dense_1 (Dense)	(None, 204)	81804
dense_2 (Dense)	(None, 1)	205
Total params: 93,609		
Trainable params: 93,609		
Non-trainable params: 0		

In [17]:

```
from sklearn.metrics import roc_curve
y_pred_keras = m.predict(X_hold).ravel()
fpr_keras, tpr_keras, thresholds_keras = roc_curve(y_hold, y_pred_keras)
```

In [18]:

```
from sklearn.metrics import auc
auc_keras = auc(fpr_keras, tpr_keras)
```

In [19]:

```
plt.figure(1)

plt.plot(fpr_keras, tpr_keras, label='Keras (area = {:.3f})'.format(auc_keras))
plt.xlabel('False positive rate')
plt.ylabel('True positive rate')
plt.title('ROC curve')
plt.legend(loc='best')
plt.show()
```

Out[19]:

<Figure size 576x396 with 0 Axes>

Out[19]:

[<matplotlib.lines.Line2D at 0x7f6f0fec1b50>]

Out[19]:

Text(0.5, 0, 'False positive rate')

Out[19]:

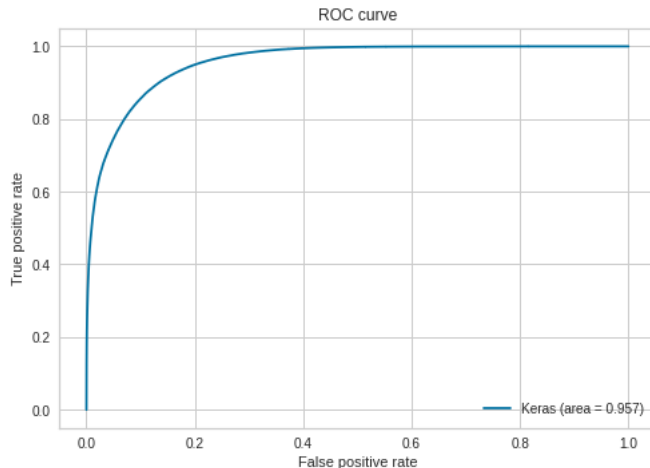
Text(0, 0.5, 'True positive rate')

Out[19]:

Text(0.5, 1.0, 'ROC curve')

Out[19]:

<matplotlib.legend.Legend at 0x7f6f0fe61550>



In [20]:

```
y_pred_keras[y_pred_keras <= 0.5] = 0.
y_pred_keras[y_pred_keras > 0.5] = 1.
```

In [21]:

```
from sklearn.metrics import confusion_matrix
import itertools

cm = confusion_matrix(y_true=y_hold, y_pred=y_pred_keras)

def plot_confusion_matrix(cm, classes,
                           normalize=False,
                           title='Confusion matrix',
                           cmap=plt.cm.Blues):
    """
    This function prints and plots the confusion matrix.
    Normalization can be applied by setting `normalize=True`.
    """
    plt.imshow(cm, interpolation='nearest', cmap=cmap)
    plt.title(title)
    plt.colorbar()
    tick_marks = np.arange(len(classes))
    plt.xticks(tick_marks, classes, rotation=45)
    plt.yticks(tick_marks, classes)

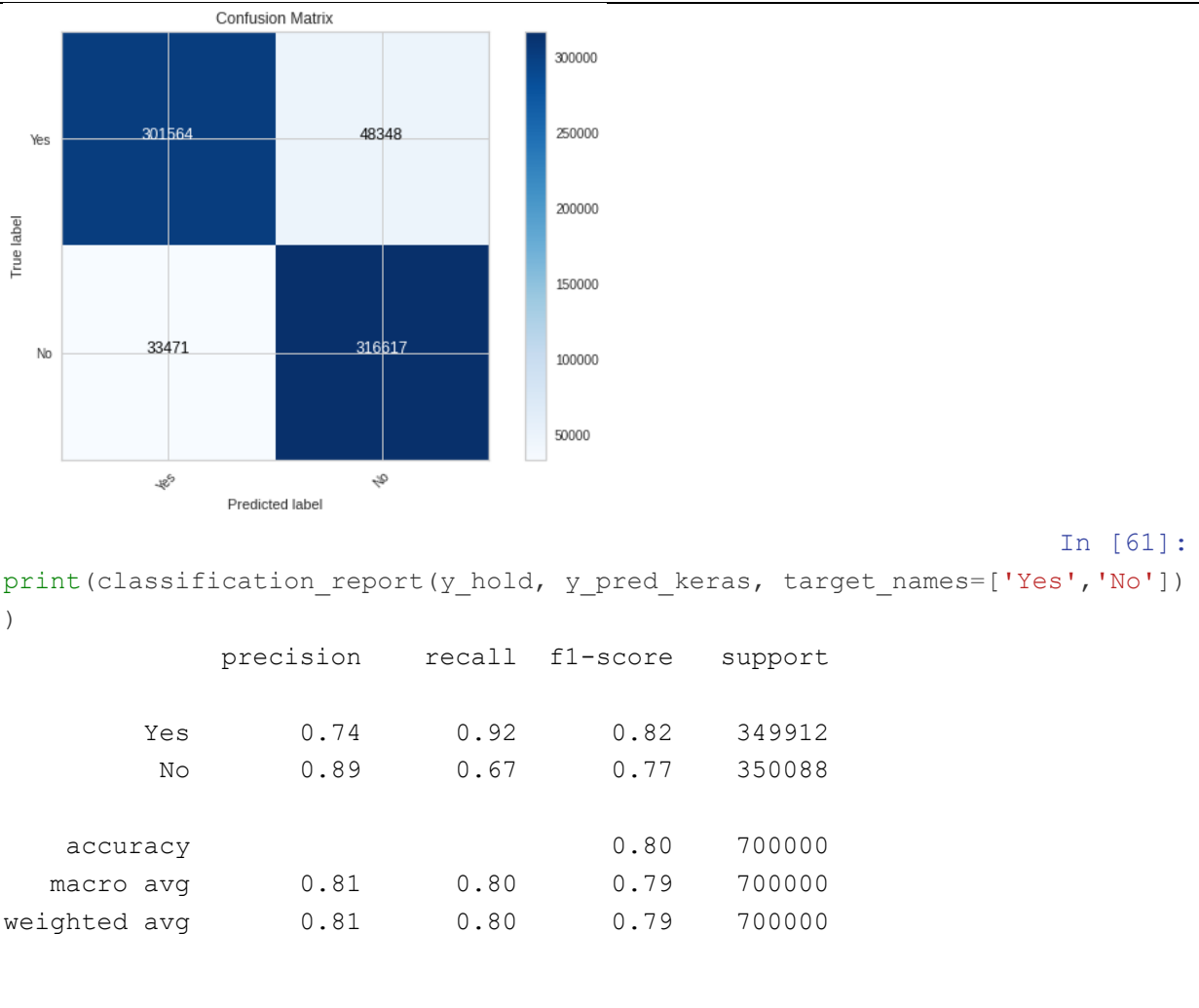
    if normalize:
        cm = cm.astype('float') / cm.sum(axis=1)[:, np.newaxis]
        print("Normalized confusion matrix")
    else:
        print('Confusion matrix, without normalization')

    print(cm)

    thresh = cm.max() / 2.
    for i, j in itertools.product(range(cm.shape[0]), range(cm.shape[1])):
        plt.text(j, i, cm[i, j],
                 horizontalalignment="center",
                 color="white" if cm[i, j] > thresh else "black")

    plt.tight_layout()
    plt.ylabel('True label')
    plt.xlabel('Predicted label')

cm_plot_labels = ['Yes', 'No']
plot_confusion_matrix(cm=cm, classes=cm_plot_labels, title='Confusion Matrix
')
Confusion matrix, without normalization
[[301564  48348]
 [ 33471 316617]]
```



6 References

1. Data set info : <https://archive.ics.uci.edu/ml/datasets/HEPMAS>
2. Article on particle physics: <https://towardsdatascience.com/how-deep-learning-can-solve-problems-in-high-energy-physics-53ed3cf5e1c5>
3. Particel physics: https://en.wikipedia.org/wiki/Particle_physics
- 4.
- 5.