Prediction of a Chemical whether it is musk or non musk, using Artificial Neural Network

Resources:

- Dataset: https://drive.google.com/file/d/1pZhzZnaPi74aKCQImSPrzrTxWzVeE0qv/view?usp=sharing
- Anaconda navigator 2019.10 :https://www.anaconda.com/distribution/ 3.7 :
- Spyder: https://www.spyder-ide.org
- pandas: https://pandas.pydata.org/pandas-docs/stable/
- Numpy: https://docs.scipy.org/doc/numpy-dev/user/quickstart.html
- Scikit-learn: http://scikit-learn.org/stable/
- Matplotlib: https://matplotlib.org/2.1.0/index.html
- Keras: https://keras.io/

Tools Used:

- Data Analysis and Preprocessing:
  - Pandas, Numpy and Scikit-learn
- Data Visualization:
  - Matplotlib
- Deep Learning Library:
  - Keras (with Tensorflow backend)

We will divide the project into 2 parts:

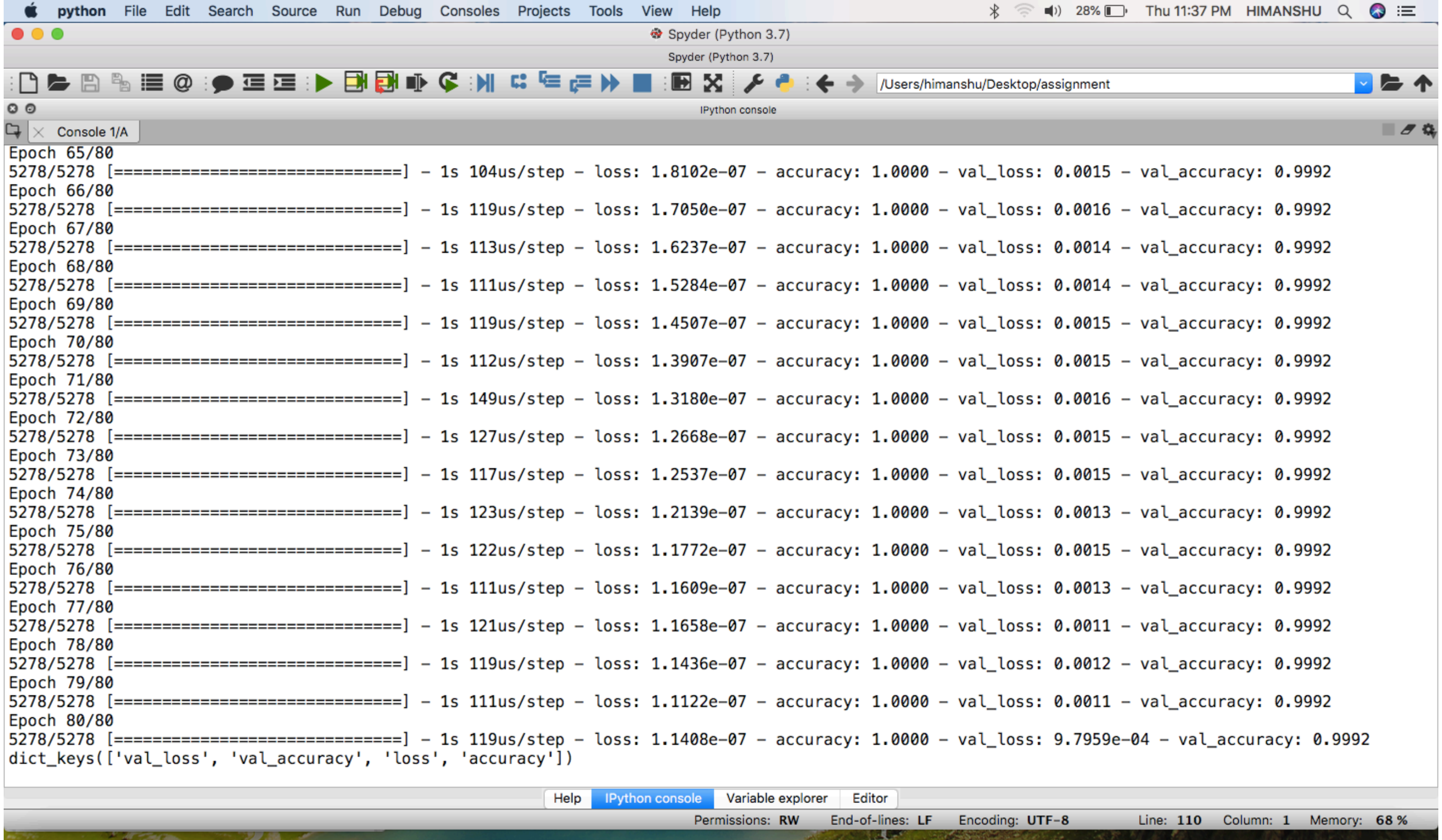
1. Data Exploration and Data Preprocessing:
    1. Description of Data
    2. Feature scaling with class StandarScaler
    3. Splitting data into training and test set
    4. Using marplotlib to visualization

Aproach:

Network Architecture:

- Input Layer with 84 Neurons(average of input and output nodes)
- First Hidden Layer with 84 Neurons and “Rectified” Activation Function
- Second Hidden Layer with 84 Neurons and “Rectified” Activation Function
- Output Layer with 1 Neurons and “Sigmoid” Activation Function
- Number of epochs 80 and batch size 20

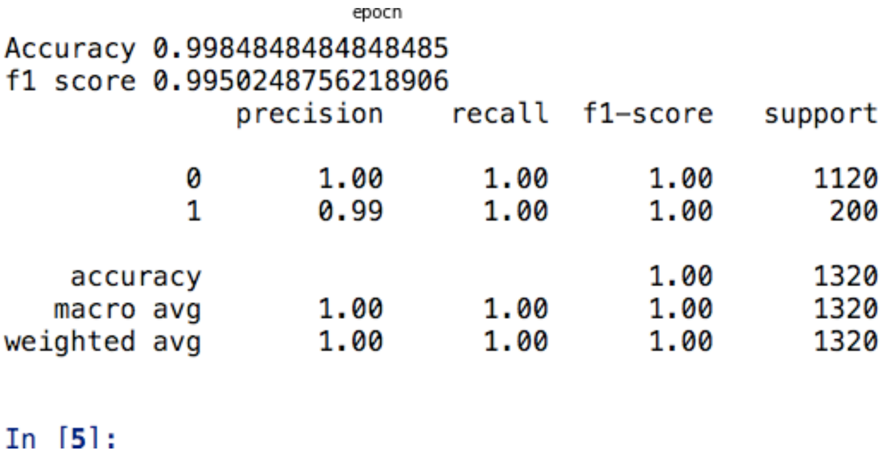
Run time :



```
Epoch 65/80
5278/5278 [==============================] - 1s 104us/step - loss: 1.8102e-07 - accuracy: 1.0000 - val_loss: 0.0015 - val_accuracy: 0.9992
Epoch 66/80
5278/5278 [==============================] - 1s 119us/step - loss: 1.7050e-07 - accuracy: 1.0000 - val_loss: 0.0016 - val_accuracy: 0.9992
Epoch 67/80
5278/5278 [==============================] - 1s 113us/step - loss: 1.6237e-07 - accuracy: 1.0000 - val_loss: 0.0014 - val_accuracy: 0.9992
Epoch 68/80
5278/5278 [==============================] - 1s 111us/step - loss: 1.5284e-07 - accuracy: 1.0000 - val_loss: 0.0014 - val_accuracy: 0.9992
Epoch 69/80
5278/5278 [==============================] - 1s 119us/step - loss: 1.4507e-07 - accuracy: 1.0000 - val_loss: 0.0015 - val_accuracy: 0.9992
Epoch 70/80
5278/5278 [==============================] - 1s 112us/step - loss: 1.3907e-07 - accuracy: 1.0000 - val_loss: 0.0015 - val_accuracy: 0.9992
Epoch 71/80
5278/5278 [==============================] - 1s 149us/step - loss: 1.3180e-07 - accuracy: 1.0000 - val_loss: 0.0016 - val_accuracy: 0.9992
Epoch 72/80
5278/5278 [==============================] - 1s 127us/step - loss: 1.2668e-07 - accuracy: 1.0000 - val_loss: 0.0015 - val_accuracy: 0.9992
Epoch 73/80
5278/5278 [==============================] - 1s 117us/step - loss: 1.2537e-07 - accuracy: 1.0000 - val_loss: 0.0015 - val_accuracy: 0.9992
Epoch 74/80
5278/5278 [==============================] - 1s 123us/step - loss: 1.2139e-07 - accuracy: 1.0000 - val_loss: 0.0013 - val_accuracy: 0.9992
Epoch 75/80
5278/5278 [==============================] - 1s 122us/step - loss: 1.1772e-07 - accuracy: 1.0000 - val_loss: 0.0015 - val_accuracy: 0.9992
Epoch 76/80
5278/5278 [==============================] - 1s 111us/step - loss: 1.1609e-07 - accuracy: 1.0000 - val_loss: 0.0013 - val_accuracy: 0.9992
Epoch 77/80
5278/5278 [==============================] - 1s 121us/step - loss: 1.1658e-07 - accuracy: 1.0000 - val_loss: 0.0011 - val_accuracy: 0.9992
Epoch 78/80
5278/5278 [==============================] - 1s 119us/step - loss: 1.1436e-07 - accuracy: 1.0000 - val_loss: 0.0012 - val_accuracy: 0.9992
Epoch 79/80
5278/5278 [==============================] - 1s 111us/step - loss: 1.1122e-07 - accuracy: 1.0000 - val_loss: 0.0011 - val_accuracy: 0.9992
Epoch 80/80
5278/5278 [==============================] - 1s 119us/step - loss: 1.1408e-07 - accuracy: 1.0000 - val_loss: 9.7959e-04 - val_accuracy: 0.9992
dict_keys(['val_loss', 'val_accuracy', 'loss', 'accuracy'])
```

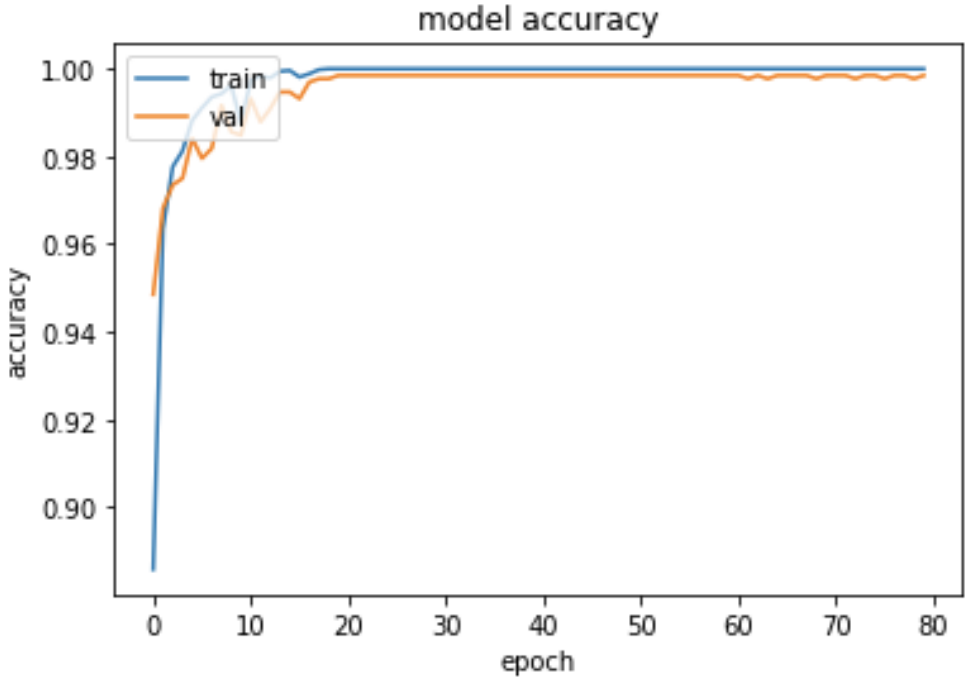
Performance:

- Accuracy: 0.9984
- F1 score :0.9950

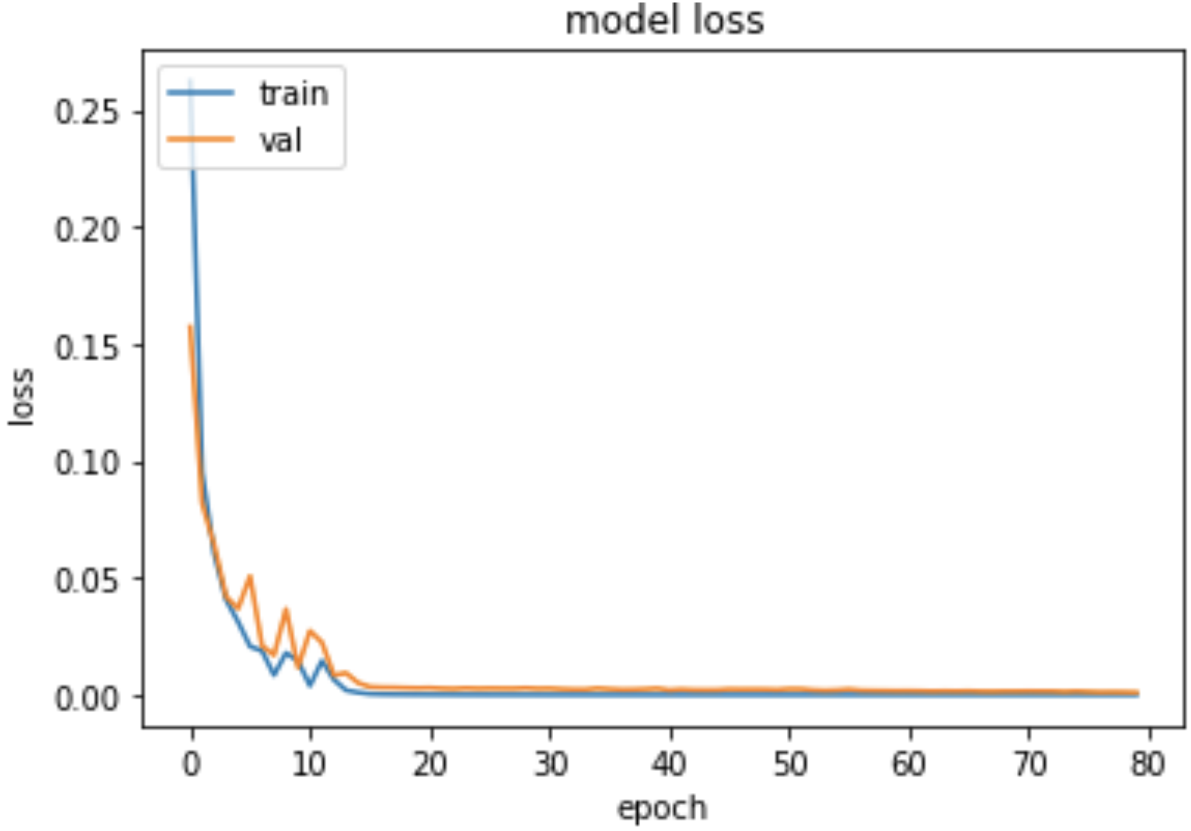


```
                                      epocn
Accuracy 0.9984848484848485
f1 score 0.9950248756218906
              precision    recall  f1-score   support

           0       1.00      1.00      1.00      1120
           1       0.99      1.00      1.00       200

    accuracy                           1.00      1320
   macro avg       1.00      1.00      1.00      1320
weighted avg       1.00      1.00      1.00      1320


In [5]:
```

Accuracy graph:



Loss Graph:


model loss
train
val
loss
0.25
0.20
0.15
0.10
0.05
0.00
0
10
20
30
40
50
60
70
80
epoch