SamipSinghalFall2021Project

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[18]:

1 2021 Fall Semester Project

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Semi - Supervised Learning Using Graph Neural Networks

References:

https://arxiv.org/pdf/1609.02907.pdf

https://github.com/danielegrattarola/spektral/blob/master/examples/node_prediction/citation_gcn.py

https://arxiv.org/abs/2006.12138

https://graphneural.network/datasets/#citation

https://arxiv.org/abs/1706.02216

1.1 Problem Statement

Solve the problem of :- Classification with 'high accuracy' in 'absence of enough labeled data'

For the purpose of this project, we would like to classify research paper into 7 different classes using only 20 samples for each class.

1.2 Outcome

GCN Outperforms FCNN FCNN F1 Score - 55% GCN F1 Score - 76% The T-SNE Plot of GCN hidden layer representation is much much less scattered as FCNN. Using only 20 labeled examples for each class , GCN outperforms FCNN by 20%.

```
import numpy as np
import os
import networkx as nx
from tensorflow.keras.utils import to_categorical
from sklearn.preprocessing import LabelEncoder
from sklearn.utils import shuffle
from sklearn.metrics import classification_report
```

```
from spektral.layers import GCSConv
from spektral.layers import GATConv
from spektral.layers import GraphSageConv
from spektral.layers import GraphConv

from tensorflow.keras.models import Model
from tensorflow.keras.layers import Input, Dropout, Dense
from tensorflow.keras import Sequential
from tensorflow.keras.optimizers import Adam
from tensorflow.keras.callbacks import TensorBoard, EarlyStopping
import tensorflow as tf
from tensorflow.keras.regularizers import 12

from collections import Counter
from sklearn.manifold import TSNE
import matplotlib.pyplot as plt
```

1.3 Data Loading and Preprocessing

```
all_data = []
all_edges = []

for root,dirs,files in os.walk('./cora'):
    for file in files:
        if '.content' in file:
            with open(os.path.join(root,file),'r') as f:
                all_data.extend(f.read().splitlines())
        elif 'cites' in file:
            with open(os.path.join(root,file),'r') as f:
                all_edges.extend(f.read().splitlines())

#Shuffle the data because the raw data is ordered based on the label random_state = 77
all_data = shuffle(all_data,random_state=random_state)
```

2 Parsing the data

```
[3]: #parse the data
labels = []
nodes = []
X = []
```

```
for i,data in enumerate(all_data):
    elements = data.split('\t')
    labels.append(elements[-1])
    X.append(elements[1:-1])
    nodes.append(elements[0])
X = np.array(X,dtype=int)
N = X.shape[0] #the number of nodes
F = X.shape[1] #the size of node features
print('X shape: ', X.shape)
#parse the edge
edge_list=[]
for edge in all_edges:
    e = edge.split('\t')
    edge_list.append((e[0],e[1]))
print('\nNumber of nodes (N): ', N)
print('\nNumber of features (F) of each node: ', F)
print('\nCategories: ', set(labels))
num classes = len(set(labels))
print('\nNumber of classes: ', num_classes)
X shape: (2708, 1433)
Number of nodes (N): 2708
Number of features (F) of each node: 1433
Categories: {'Theory', 'Case_Based', 'Genetic_Algorithms',
'Probabilistic_Methods', 'Reinforcement_Learning', 'Rule_Learning',
'Neural_Networks'}
```

3 Select examples for training, validation, and test then set the mask

Number of classes: 7

```
for i in range(len(labels)):
        label = labels[i]
        if label_counter[label]<limit:</pre>
            #add the example to the training data
            train_idx.append(i)
            label_counter[label]+=1
        #exit the loop once we found 20 examples for each class
        if all(count == limit for count in label_counter.values()):
            break
    #get the indices that do not go to traning data
    rest_idx = [x for x in range(len(labels)) if x not in train_idx]
    #get the first val_num
    val_idx = rest_idx[:val_num]
    test_idx = rest_idx[val_num:(val_num+test_num)]
    return train_idx, val_idx,test_idx
train_idx,val_idx,test_idx = limit_data(labels)
```

```
[5]: #set the mask
train_mask = np.zeros((N,),dtype=bool)
train_mask[train_idx] = True

val_mask = np.zeros((N,),dtype=bool)
val_mask[val_idx] = True

test_mask = np.zeros((N,),dtype=bool)
test_mask[test_idx] = True
```

4 Data Distribution

'Rule_Learning': 20})

```
[8]: print("Validation Data Distribution: \n{}".format(Counter([labels[i] for i in_ oval_idx])))

Validation Data Distribution:
Counter({'Neural_Networks': 172, 'Genetic_Algorithms': 78, 'Probabilistic_Methods': 72, 'Theory': 63, 'Case_Based': 58, 'Reinforcement_Learning': 35, 'Rule_Learning': 22})
```

5 Convert the labels to one hot encoding

```
[9]: def encode_label(labels):
    label_encoder = LabelEncoder()
    labels = label_encoder.fit_transform(labels)
    labels = to_categorical(labels)
    return labels, label_encoder.classes_

labels_encoded, classes = encode_label(labels)
```

6 Build a graph on NetworkX using the obtained nodes and edges list

```
[10]: #build the graph
G = nx.Graph()
G.add_nodes_from(nodes)
G.add_edges_from(edge_list)

#obtain the adjacency matrix (A)
A = nx.adjacency_matrix(G)
print('Graph info: ', nx.info(G))
```

Graph info: Name: Type: Graph

Number of nodes: 2708 Number of edges: 5278 Average degree: 3.8981

7 Building and Training Graph Convolutional Networks

```
# Preprocessing operations
A = GraphSageConv.preprocess(A).astype('f4')
# Model definition
X_in = Input(shape=(F, ))
fltr_in = Input((N, ), sparse=True)
dropout_1 = Dropout(dropout)(X_in)
graph_conv_1 = GraphSageConv(channels,
                          activation='relu',
                         kernel_regularizer=12(12_reg),
                         use_bias=False)([dropout_1, fltr_in])
dropout_2 = Dropout(dropout)(graph_conv_1)
graph_conv_2 = GraphSageConv(num_classes,
                         activation='softmax',
                         use_bias=False)([dropout_2, fltr_in])
# Build model
model = Model(inputs=[X_in, fltr_in], outputs=graph_conv_2)
optimizer = Adam(learning_rate=learning_rate)
model.compile(optimizer=optimizer,
              loss='categorical_crossentropy',
              weighted_metrics=['acc'])
model.summary()
tbCallBack_GCN = tf.keras.callbacks.TensorBoard(
    log_dir='./Tensorboard_GCN_cora',
callback_GCN = [tbCallBack_GCN]
Model: "model_4"
```

Layer (type)	Output Shape	Param #	Connected to
input_11 (InputLayer)	[(None, 1433)]	0	[]
<pre>dropout_9 (Dropout) ['input_11[0][0]']</pre>	(None, 1433)	0	
<pre>input_12 (InputLayer)</pre>	[(None, 2708)]	0	
<pre>graph_sage_conv_4 (GraphSageCo ['dropout_9[0][0]', nv) 'input_12[0][0]']</pre>	(None, 16)	45856	

```
['graph_sage_conv_4[0][0]']
    graph_sage_conv_5 (GraphSageCo (None, 7)
                                          224
    ['dropout_10[0][0]',
    nv)
    'input_12[0][0]']
   ============
   Total params: 46,080
   Trainable params: 46,080
   Non-trainable params: 0
[26]: # Train model
    validation_data = ([X, A], labels_encoded, val_mask)
    model.fit([X, A],
           labels_encoded,
           sample_weight=train_mask,
           epochs=epochs,
           batch_size=N,
           validation_data=validation_data,
           shuffle=False,
           callbacks=[
              EarlyStopping(patience=es_patience, restore_best_weights=True),
              tbCallBack GCN
           1)
   Epoch 1/200
   val_loss: 0.3488 - val_acc: 0.2920
   Epoch 2/200
   1/1 [============ ] - Os 280ms/step - loss: 0.1052 - acc:
   0.3143 - val_loss: 0.3400 - val_acc: 0.4100
   Epoch 3/200
   0.4500 - val_loss: 0.3298 - val_acc: 0.4580
   Epoch 4/200
   1/1 [=========== ] - Os 365ms/step - loss: 0.0957 - acc:
   0.5500 - val_loss: 0.3175 - val_acc: 0.5260
   Epoch 5/200
   0.6714 - val_loss: 0.3094 - val_acc: 0.5780
   Epoch 6/200
```

(None, 16)

0

dropout_10 (Dropout)

```
0.7500 - val_loss: 0.3043 - val_acc: 0.6440
Epoch 7/200
1/1 [============ ] - Os 283ms/step - loss: 0.0902 - acc:
0.7571 - val_loss: 0.3019 - val_acc: 0.6700
Epoch 8/200
0.8500 - val_loss: 0.3011 - val_acc: 0.6820
Epoch 9/200
1/1 [=========== ] - Os 354ms/step - loss: 0.0900 - acc:
0.8071 - val_loss: 0.2997 - val_acc: 0.6800
Epoch 10/200
0.8643 - val_loss: 0.2981 - val_acc: 0.6840
Epoch 11/200
1/1 [=========== ] - Os 282ms/step - loss: 0.0876 - acc:
0.8857 - val_loss: 0.2961 - val_acc: 0.6780
Epoch 12/200
0.8714 - val_loss: 0.2939 - val_acc: 0.6800
Epoch 13/200
0.8786 - val_loss: 0.2917 - val_acc: 0.6880
Epoch 14/200
0.9143 - val_loss: 0.2905 - val_acc: 0.6840
Epoch 15/200
0.8571 - val_loss: 0.2899 - val_acc: 0.6880
Epoch 16/200
0.9286 - val_loss: 0.2896 - val_acc: 0.6720
Epoch 17/200
0.8857 - val_loss: 0.2886 - val_acc: 0.6660
Epoch 18/200
0.9429 - val loss: 0.2878 - val acc: 0.6640
Epoch 19/200
0.9429 - val_loss: 0.2867 - val_acc: 0.6680
Epoch 20/200
1/1 [=========== ] - Os 281ms/step - loss: 0.0786 - acc:
0.9643 - val_loss: 0.2849 - val_acc: 0.6700
Epoch 21/200
0.9214 - val_loss: 0.2831 - val_acc: 0.6680
Epoch 22/200
```

```
0.9500 - val_loss: 0.2805 - val_acc: 0.6820
Epoch 23/200
0.9071 - val_loss: 0.2781 - val_acc: 0.6980
Epoch 24/200
0.9286 - val_loss: 0.2754 - val_acc: 0.7100
Epoch 25/200
1/1 [============ ] - Os 288ms/step - loss: 0.0759 - acc:
0.9357 - val_loss: 0.2732 - val_acc: 0.7160
Epoch 26/200
0.9429 - val_loss: 0.2719 - val_acc: 0.7140
Epoch 27/200
1/1 [=========== ] - Os 286ms/step - loss: 0.0739 - acc:
0.9500 - val_loss: 0.2716 - val_acc: 0.7180
Epoch 28/200
0.9429 - val_loss: 0.2723 - val_acc: 0.7060
Epoch 29/200
0.9571 - val_loss: 0.2727 - val_acc: 0.6940
Epoch 30/200
0.9571 - val_loss: 0.2726 - val_acc: 0.7000
Epoch 31/200
0.9286 - val_loss: 0.2716 - val_acc: 0.7080
0.9357 - val_loss: 0.2693 - val_acc: 0.7180
Epoch 33/200
0.9357 - val_loss: 0.2663 - val_acc: 0.7260
Epoch 34/200
0.9500 - val_loss: 0.2633 - val_acc: 0.7460
Epoch 35/200
0.9357 - val_loss: 0.2616 - val_acc: 0.7480
Epoch 36/200
1/1 [=========== ] - Os 281ms/step - loss: 0.0696 - acc:
0.9643 - val_loss: 0.2605 - val_acc: 0.7440
Epoch 37/200
1/1 [=========== ] - Os 271ms/step - loss: 0.0711 - acc:
0.9357 - val_loss: 0.2608 - val_acc: 0.7340
Epoch 38/200
```

```
0.9429 - val_loss: 0.2604 - val_acc: 0.7360
Epoch 39/200
1/1 [============ ] - Os 276ms/step - loss: 0.0691 - acc:
0.9429 - val_loss: 0.2614 - val_acc: 0.7140
Epoch 40/200
0.9429 - val_loss: 0.2623 - val_acc: 0.7200
Epoch 41/200
1/1 [=========== ] - Os 313ms/step - loss: 0.0705 - acc:
0.9286 - val_loss: 0.2643 - val_acc: 0.7080
Epoch 42/200
1/1 [============ ] - Os 300ms/step - loss: 0.0689 - acc:
0.9286 - val_loss: 0.2653 - val_acc: 0.7020
Epoch 43/200
0.9071 - val_loss: 0.2644 - val_acc: 0.7260
Epoch 44/200
0.9357 - val_loss: 0.2630 - val_acc: 0.7440
Epoch 45/200
0.9214 - val_loss: 0.2620 - val_acc: 0.7440
Epoch 46/200
0.9500 - val_loss: 0.2607 - val_acc: 0.7520
Epoch 47/200
0.9714 - val_loss: 0.2595 - val_acc: 0.7580
0.9714 - val_loss: 0.2593 - val_acc: 0.7520
Epoch 49/200
0.9429 - val_loss: 0.2610 - val_acc: 0.7420
Epoch 50/200
0.9143 - val_loss: 0.2636 - val_acc: 0.7280
Epoch 51/200
0.9429 - val_loss: 0.2657 - val_acc: 0.7200
Epoch 52/200
1/1 [=========== ] - Os 276ms/step - loss: 0.0696 - acc:
0.9286 - val_loss: 0.2659 - val_acc: 0.7140
Epoch 53/200
1/1 [============ ] - Os 269ms/step - loss: 0.0692 - acc:
0.9571 - val_loss: 0.2659 - val_acc: 0.7180
Epoch 54/200
```

```
0.9143 - val_loss: 0.2641 - val_acc: 0.7220
    Epoch 55/200
    0.9571 - val_loss: 0.2623 - val_acc: 0.7320
    Epoch 56/200
    0.9429 - val loss: 0.2609 - val acc: 0.7460
    Epoch 57/200
    0.9143 - val_loss: 0.2603 - val_acc: 0.7540
    Epoch 58/200
    0.9643 - val_loss: 0.2603 - val_acc: 0.7500
[26]: <keras.callbacks.History at 0x7fdb2e4da290>
[21]: # Evaluate model
    X te = X[test mask]
    A_te = A[test_mask,:][:,test_mask]
    y_te = labels_encoded[test_mask]
    y_pred = model.predict([X_te, A_te], batch_size=N)
    report = classification_report(np.argmax(y_te,axis=1), np.
     →argmax(y_pred,axis=1), target_names=classes)
    print('GCN Classification Report: \n {}'.format(report))
             -----
          ValueError
                                           Traceback (most recent call_
     →last)
          <ipython-input-21-3f83555e3485> in <module>
            4 y_te = labels_encoded[test_mask]
       ----> 6 y_pred = model.predict([X_te, A_te], batch_size=N)
            7 report = classification_report(np.argmax(y_te,axis=1), np.
     →argmax(y_pred,axis=1), target_names=classes)
            8 print('GCN Classification Report: \n {}'.format(report))
          ~/opt/anaconda3/lib/python3.7/site-packages/keras/utils/traceback_utils.
     →py in error_handler(*args, **kwargs)
           65
                except Exception as e: # pylint: disable=broad-except
                  filtered_tb = _process_traceback_frames(e.__traceback__)
           66
                  raise e.with_traceback(filtered_tb) from None
       ---> 67
           68
                finally:
```

```
del filtered_tb
```

```
~/opt/anaconda3/lib/python3.7/site-packages/tensorflow/python/framework/

→func_graph.py in autograph_handler(*args, **kwargs)
      1127
                     except Exception as e: # pylint:disable=broad-except
                       if hasattr(e, "ag_error_metadata"):
      1128
  -> 1129
                         raise e.ag_error_metadata.to_exception(e)
      1130
                       else:
      1131
                         raise
       ValueError: in user code:
       File "/Users/samipsinghal/opt/anaconda3/lib/python3.7/site-packages/
→keras/engine/training.py", line 1621, in predict_function *
           return step function(self, iterator)
       File "/Users/samipsinghal/opt/anaconda3/lib/python3.7/site-packages/
→keras/engine/training.py", line 1611, in step_function **
           outputs = model.distribute strategy.run(run step, args=(data,))
       File "/Users/samipsinghal/opt/anaconda3/lib/python3.7/site-packages/
→keras/engine/training.py", line 1604, in run_step **
           outputs = model.predict_step(data)
       File "/Users/samipsinghal/opt/anaconda3/lib/python3.7/site-packages/
→keras/engine/training.py", line 1572, in predict_step
           return self(x, training=False)
      File "/Users/samipsinghal/opt/anaconda3/lib/python3.7/site-packages/
→keras/utils/traceback_utils.py", line 67, in error_handler
           raise e.with_traceback(filtered_tb) from None
       File "/Users/samipsinghal/opt/anaconda3/lib/python3.7/site-packages/
→keras/engine/input_spec.py", line 263, in assert_input_compatibility
```

→expected shape=(None, 2708), found shape=(None, 1000)

raise ValueError(f'Input {input index} of layer "{layer name}" is '

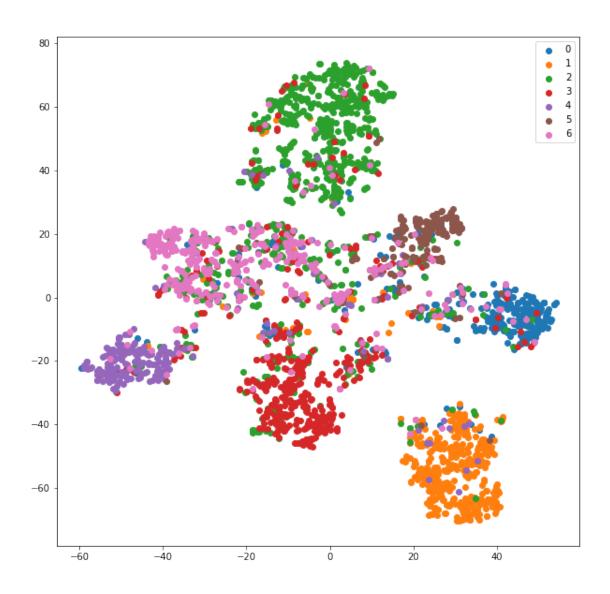
ValueError: Input 1 of layer "model_2" is incompatible with the layer:

8 Get hidden layer representation for GCN

```
[27]: layer_outputs = [layer.output for layer in model.layers]
activation_model = Model(inputs=model.input, outputs=layer_outputs)
activations = activation_model.predict([X,A],batch_size=N)

#Get t-SNE Representation
#get the hidden layer representation after the first GCN layer
```

```
x_tsne = TSNE(n_components=2).fit_transform(activations[3])
     /Users/samipsinghal/opt/anaconda3/lib/python3.7/site-
     packages/sklearn/manifold/_t_sne.py:783: FutureWarning: The default
     initialization in TSNE will change from 'random' to 'pca' in 1.2.
       FutureWarning,
     /Users/samipsinghal/opt/anaconda3/lib/python3.7/site-
     packages/sklearn/manifold/_t_sne.py:793: FutureWarning: The default learning
     rate in TSNE will change from 200.0 to 'auto' in 1.2.
       FutureWarning,
[28]: def plot_tSNE(labels_encoded,x_tsne):
          color_map = np.argmax(labels_encoded, axis=1)
          plt.figure(figsize=(10,10))
          for cl in range(num_classes):
              indices = np.where(color_map==cl)
              indices = indices[0]
              plt.scatter(x_tsne[indices,0], x_tsne[indices, 1], label=cl)
          plt.legend()
          plt.show()
      plot_tSNE(labels_encoded,x_tsne)
```



9 Comparison to Fully-Connected Neural Networks

```
activation=tf.nn.relu,
                   kernel_regularizer=tf.keras.regularizers.12(12_reg))
model_fnn.add(Dropout(0.5))
model_fnn.add(Dense(256, activation=tf.nn.relu))
model_fnn.add(Dropout(0.5))
model_fnn.add(Dense(num_classes, activation=tf.keras.activations.softmax))
model_fnn.compile(optimizer=optimizer,
             loss='categorical_crossentropy',
             weighted_metrics=['acc'])
#define TensorBoard
tbCallBack_FNN = TensorBoard(
    log_dir='./Tensorboard_FNN_cora',
#Train model
validation_data_fnn = (X, labels_encoded, val_mask)
model_fnn.fit(
               X, labels_encoded,
               sample weight=train mask,
               epochs=epochs,
               batch_size=N,
               validation_data=validation_data_fnn,
               shuffle=False,
               callbacks=[
                 EarlyStopping(patience=es_patience, _
 →restore_best_weights=True),
                 tbCallBack FNN
         ])
Epoch 1/200
```

```
Epoch 6/200
   0.8286 - val_loss: 0.2614 - val_acc: 0.6080
   Epoch 7/200
   0.8786 - val_loss: 0.2545 - val_acc: 0.5960
   Epoch 8/200
   1/1 [============ ] - Os 111ms/step - loss: 0.0469 - acc:
   0.9429 - val_loss: 0.2707 - val_acc: 0.5700
   Epoch 9/200
   0.9500 - val_loss: 0.2940 - val_acc: 0.5720
   Epoch 10/200
   1/1 [=========== ] - Os 104ms/step - loss: 0.0415 - acc:
   0.9929 - val_loss: 0.3226 - val_acc: 0.5600
   Epoch 11/200
   0.9786 - val_loss: 0.3547 - val_acc: 0.5380
   Epoch 12/200
   0.9786 - val_loss: 0.3728 - val_acc: 0.5360
   Epoch 13/200
   0.9929 - val_loss: 0.3805 - val_acc: 0.5320
   Epoch 14/200
   0.9857 - val_loss: 0.3795 - val_acc: 0.5420
   0.9786 - val_loss: 0.3792 - val_acc: 0.5520
   Epoch 16/200
   - val_loss: 0.3761 - val_acc: 0.5660
   Epoch 17/200
   1.0000 - val loss: 0.3773 - val acc: 0.5580
[31]: <keras.callbacks.History at 0x7fdb0d4a1ed0>
[32]: # Evaluate model
   y_pred = model_fnn.predict(X_te)
   report = classification_report(np.argmax(y_te,axis=1), np.
   →argmax(y_pred,axis=1), target_names=classes)
   print('FCNN Classification Report: \n {}'.format(report))
   FCNN Classification Report:
```

0.8071 - val_loss: 0.2881 - val_acc: 0.6120

precision recall f1-score

support

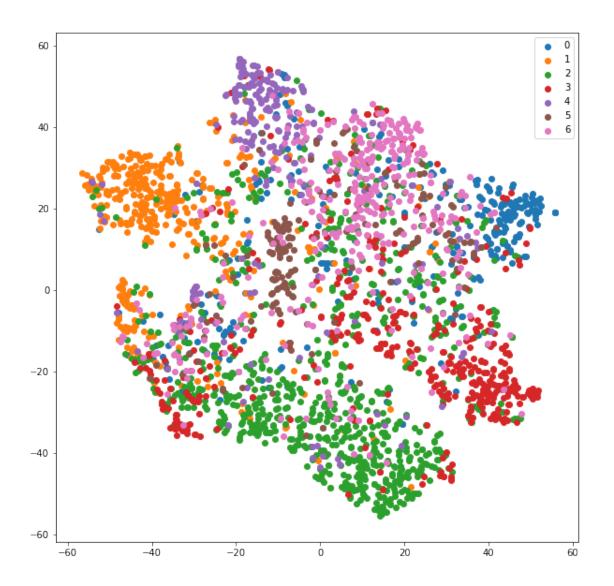
```
Case_Based
                              0.50
                                        0.56
                                                  0.53
                                                              114
    Genetic_Algorithms
                              0.75
                                        0.71
                                                  0.73
                                                              156
       Neural_Networks
                             0.72
                                        0.54
                                                  0.62
                                                              290
Probabilistic Methods
                             0.70
                                        0.50
                                                  0.58
                                                              172
Reinforcement_Learning
                             0.54
                                        0.52
                                                  0.53
                                                               85
         Rule_Learning
                              0.42
                                        0.60
                                                  0.49
                                                               60
                              0.34
                                        0.60
                                                  0.44
                Theory
                                                              123
              accuracy
                                                  0.57
                                                             1000
                                                  0.56
             macro avg
                              0.57
                                        0.58
                                                             1000
          weighted avg
                              0.62
                                        0.57
                                                  0.58
                                                             1000
```

```
[33]: layer_outputs = [layer.output for layer in model_fnn.layers]
activation_model = Model(inputs=model_fnn.input, outputs=layer_outputs)
activations = activation_model.predict([X])
```

```
[34]: x_tsne = TSNE(n_components=2).fit_transform(activations[3]) plot_tSNE(labels_encoded,x_tsne)
```

/Users/samipsinghal/opt/anaconda3/lib/python3.7/site-packages/sklearn/manifold/_t_sne.py:783: FutureWarning: The default initialization in TSNE will change from 'random' to 'pca' in 1.2. FutureWarning,

/Users/samipsinghal/opt/anaconda3/lib/python3.7/site-packages/sklearn/manifold/_t_sne.py:793: FutureWarning: The default learning rate in TSNE will change from 200.0 to 'auto' in 1.2. FutureWarning,



[]: