Node Classification using Graph Convolutional Networks

200

This node classification task uses CORA dataset from https://lings.soe.ucsc.edu/data

The dataset consists of 2708 nodes which correspond to scientific publications.

The nodes are classified into **7** categories indicating the topics of each document.

The edges indicate whether a document is cited by the other or vice versa.

Each node has 1433 features which is described by a 0/1-valued vector, indicating the bag-of-words from the dictionary.

This is an undirected graph problem

```
In [ ]: #importing dependencies
        import numpy as np
        import os
        import networkx as nx
        from 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 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
```

Data Loading and Preprocessing

We are going to use the edges connecting the (from file cora.cites).

The nodes are loaded from file cora.content.

In cora.content file:

The first element indicates the node name

The **second** until the last second elements indicate the **node features**

The last element indicates the label of that particular node

In cora.cites file:

Each line indicates the tuple of connected nodes

Parsing the data

```
In [ ]: #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: {'Probabilistic_Methods', 'Theory', 'Neural_Networks', 'Reinforcement_Learning', 'Case_Based',
        'Rule_Learning', 'Genetic_Algorithms'}
        Number of classes: 7
```

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

```
#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)

In []: #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
```

Show Data Distribution

Convert the labels to one hot encoding

```
In [ ]: 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)
```

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

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

#bbtain 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
```

Building and Training Graph Convolutional Networks

```
In [ ]: # Parameters
        channels = 16
                               # Number of channels in the first layer
        dropout = 0.5  # Dropout rate for the features
12 reg = 5e-4  # L2 regularization rate
        12_{reg} = 5e-4
                               # L2 regularization rate
        es_patience = 100

# Number of training epochs
# Patience for a
        learning_rate = 1e-2  # Learning rate
                               # Patience for early stopping
        # Preprocessing operations
        A = GraphConv.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 = GraphConv(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 = GraphConv(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(lr=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"
        Layer (type)
                                        Output Shape
                                                            Param #
        input_1 (InputLayer)
                                        [(None, 1433)]
        dropout (Dropout)
                                        (None, 1433)
                                                            0
                                                                        input_1[0][0]
                                        [(None, 2708)]
        input_2 (InputLayer)
                                                            0
                                                            22928
        graph_conv (GraphConv)
                                        (None, 16)
                                                                        dropout[0][0]
                                                                        input_2[0][0]
        dropout_1 (Dropout)
                                        (None, 16)
                                                                        graph_conv[0][0]
        graph_conv_1 (GraphConv)
                                        (None, 7)
                                                                        dropout_1[0][0]
                                                            112
                                                                        input_2[0][0]
        ______
        Total params: 23,040
        Trainable params: 23,040
        Non-trainable params: 0
In [ ]: # 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
])
```

```
Epoch 1/200
1/1 [=============] - 0s 470ms/step - loss: 0.1162 - acc: 0.1143 - val_loss: 0.3629 - val_ac
c: 0.4000
Epoch 2/200
n_batch_end) is slow compared to the batch update (0.205158). Check your callbacks.
c: 0.5460
Epoch 3/200
c: 0.6360
Epoch 4/200
1/1 [============ ] - 0s 320ms/step - loss: 0.0954 - acc: 0.7000 - val_loss: 0.3264 - val_ac
c: 0.6620
Epoch 5/200
1/1 [============= ] - 0s 351ms/step - loss: 0.0896 - acc: 0.7286 - val_loss: 0.3175 - val_ac
c: 0.6740
Epoch 6/200
1/1 [=========== ] - 0s 278ms/step - loss: 0.0836 - acc: 0.8214 - val loss: 0.3088 - val ac
c: 0.6720
Epoch 7/200
1/1 [==============] - 0s 305ms/step - loss: 0.0812 - acc: 0.7857 - val_loss: 0.3005 - val_ac
c: 0.6860
Fnoch 8/200
c: 0.7000
Epoch 9/200
c: 0.7080
Epoch 10/200
c: 0.7260
Epoch 11/200
c: 0.7300
Epoch 12/200
1/1 [===========] - 0s 328ms/step - loss: 0.0662 - acc: 0.9143 - val_loss: 0.2595 - val_ac
c: 0.7320
Epoch 13/200
c: 0.7420
Epoch 14/200
1/1 [============= ] - 0s 331ms/step - loss: 0.0618 - acc: 0.9357 - val_loss: 0.2461 - val_ac
c: 0.7460
Epoch 15/200
c: 0.7500
Epoch 16/200
c: 0.7600
Epoch 17/200
1/1 [=========== ] - 0s 278ms/step - loss: 0.0598 - acc: 0.9286 - val loss: 0.2306 - val ac
c: 0.7640
Epoch 18/200
c: 0.7620
Epoch 19/200
1/1 [=========== ] - 0s 402ms/step - loss: 0.0570 - acc: 0.9214 - val loss: 0.2239 - val ac
c: 0.7640
Epoch 20/200
c: 0.7600
Epoch 21/200
1/1 [============= ] - 0s 340ms/step - loss: 0.0565 - acc: 0.8929 - val_loss: 0.2181 - val_ac
c: 0.7600
Epoch 22/200
1/1 [============= ] - 0s 268ms/step - loss: 0.0547 - acc: 0.9143 - val_loss: 0.2148 - val_ac
c: 0.7600
Epoch 23/200
1/1 [===========] - 0s 256ms/step - loss: 0.0529 - acc: 0.9286 - val_loss: 0.2117 - val_ac
c: 0.7620
```

```
Epoch 24/200
1/1 [============= ] - 0s 290ms/step - loss: 0.0534 - acc: 0.9071 - val_loss: 0.2085 - val_ac
c: 0.7640
Epoch 25/200
c: 0.7620
Epoch 26/200
1/1 [==========] - 0s 228ms/step - loss: 0.0484 - acc: 0.9500 - val_loss: 0.2028 - val_ac
c: 0.7720
Epoch 27/200
1/1 [============= ] - 0s 231ms/step - loss: 0.0485 - acc: 0.9357 - val_loss: 0.2001 - val_ac
c: 0.7740
Epoch 28/200
1/1 [=========== ] - 0s 248ms/step - loss: 0.0490 - acc: 0.9500 - val loss: 0.1975 - val ac
c: 0.7740
Epoch 29/200
c: 0.7660
Epoch 30/200
1/1 [============= ] - 0s 239ms/step - loss: 0.0505 - acc: 0.9357 - val_loss: 0.1928 - val_ac
c: 0.7600
Epoch 31/200
c: 0.7620
Epoch 32/200
c: 0.7620
Epoch 33/200
c: 0.7620
Epoch 34/200
1/1 [============= ] - 0s 185ms/step - loss: 0.0438 - acc: 0.9643 - val_loss: 0.1873 - val_ac
c: 0.7640
Epoch 35/200
c: 0.7680
Epoch 36/200
c: 0.7780
Epoch 37/200
c: 0.7800
Epoch 38/200
c: 0.7900
Epoch 39/200
1/1 [============ ] - 0s 406ms/step - loss: 0.0441 - acc: 0.9286 - val loss: 0.1805 - val ac
c: 0.7880
Epoch 40/200
1/1 [===========] - 0s 210ms/step - loss: 0.0408 - acc: 0.9714 - val_loss: 0.1798 - val_ac
c: 0.7820
Epoch 41/200
1/1 [============= ] - 0s 187ms/step - loss: 0.0427 - acc: 0.9429 - val_loss: 0.1787 - val_ac
c: 0.7760
Epoch 42/200
c: 0.7780
Epoch 43/200
c: 0.7740
Epoch 44/200
c: 0.7680
Epoch 45/200
c: 0.7740
Epoch 46/200
c: 0.7700
Epoch 47/200
1/1 [================] - 0s 200ms/step - loss: 0.0414 - acc: 0.9214 - val_loss: 0.1731 - val_ac
```

```
c: 0.7700
Epoch 48/200
c: 0.7880
Epoch 49/200
1/1 [===========] - 0s 201ms/step - loss: 0.0386 - acc: 0.9786 - val_loss: 0.1679 - val_ac
c: 0.7860
Epoch 50/200
1/1 [===========] - 0s 208ms/step - loss: 0.0415 - acc: 0.9500 - val_loss: 0.1663 - val_ac
c: 0.7900
Epoch 51/200
c: 0.7880
Epoch 52/200
1/1 [============= ] - 0s 193ms/step - loss: 0.0402 - acc: 0.9500 - val_loss: 0.1659 - val_ac
c: 0.7840
Epoch 53/200
c: 0.7780
Epoch 54/200
c: 0.7720
Epoch 55/200
1/1 [=========== ] - 0s 207ms/step - loss: 0.0377 - acc: 0.9571 - val loss: 0.1712 - val ac
c: 0.7680
Epoch 56/200
c: 0.7680
Epoch 57/200
1/1 [===========] - 0s 211ms/step - loss: 0.0362 - acc: 0.9571 - val_loss: 0.1708 - val_ac
c: 0.7720
Epoch 58/200
c: 0.7880
Epoch 59/200
c: 0.7840
Epoch 60/200
c: 0.7840
Epoch 61/200
c: 0.7900
Epoch 62/200
c: 0.7800
Epoch 63/200
1/1 [============= ] - 0s 194ms/step - loss: 0.0347 - acc: 0.9643 - val_loss: 0.1615 - val_ac
c: 0.7780
Epoch 64/200
c: 0.7700
Epoch 65/200
1/1 [============== ] - 0s 197ms/step - loss: 0.0362 - acc: 0.9500 - val_loss: 0.1620 - val_ac
c: 0.7700
Epoch 66/200
1/1 [============= ] - 0s 180ms/step - loss: 0.0380 - acc: 0.9286 - val_loss: 0.1627 - val_ac
c: 0.7640
Epoch 67/200
c: 0.7640
Epoch 68/200
1/1 [============ ] - 0s 200ms/step - loss: 0.0356 - acc: 0.9500 - val loss: 0.1636 - val ac
c: 0.7640
Epoch 69/200
c: 0.7700
Epoch 70/200
1/1 [============= ] - 0s 193ms/step - loss: 0.0347 - acc: 0.9429 - val_loss: 0.1613 - val_ac
c: 0.7780
Epoch 71/200
```

```
c: 0.7820
Epoch 72/200
1/1 [============= ] - 0s 191ms/step - loss: 0.0335 - acc: 0.9857 - val_loss: 0.1598 - val_ac
c: 0.7820
Epoch 73/200
c: 0.7840
Epoch 74/200
c: 0.7780
Epoch 75/200
1/1 [============= ] - 0s 188ms/step - loss: 0.0344 - acc: 0.9643 - val_loss: 0.1578 - val_ac
c: 0.7700
Epoch 76/200
1/1 [============= ] - 0s 207ms/step - loss: 0.0322 - acc: 0.9714 - val_loss: 0.1586 - val_ac
c: 0.7620
Epoch 77/200
1/1 [=========== ] - 0s 197ms/step - loss: 0.0329 - acc: 0.9571 - val loss: 0.1599 - val ac
c: 0.7600
Epoch 78/200
1/1 [=============] - 0s 218ms/step - loss: 0.0339 - acc: 0.9643 - val_loss: 0.1615 - val_ac
c: 0.7580
Fnoch 79/200
c: 0.7540
Epoch 80/200
c: 0.7480
Epoch 81/200
c: 0.7560
Epoch 82/200
c: 0.7720
Epoch 83/200
1/1 [============= ] - 0s 186ms/step - loss: 0.0329 - acc: 0.9643 - val_loss: 0.1594 - val_ac
c: 0.7820
Epoch 84/200
c: 0.7780
Epoch 85/200
1/1 [============= ] - 0s 188ms/step - loss: 0.0317 - acc: 0.9643 - val_loss: 0.1547 - val_ac
c: 0.7820
Epoch 86/200
c: 0.7820
Epoch 87/200
c: 0.7720
Epoch 88/200
1/1 [=========== ] - 0s 183ms/step - loss: 0.0306 - acc: 0.9857 - val loss: 0.1556 - val ac
c: 0.7740
Epoch 89/200
c: 0.7720
Epoch 90/200
1/1 [============ ] - 0s 186ms/step - loss: 0.0312 - acc: 0.9571 - val loss: 0.1550 - val ac
c: 0.7740
Epoch 91/200
c: 0.7740
Epoch 92/200
1/1 [============= ] - 0s 189ms/step - loss: 0.0270 - acc: 0.9929 - val_loss: 0.1524 - val_ac
c: 0.7760
Epoch 93/200
1/1 [============= ] - 0s 186ms/step - loss: 0.0299 - acc: 0.9786 - val_loss: 0.1507 - val_ac
c: 0.7780
Epoch 94/200
c: 0.7780
```

```
Epoch 95/200
1/1 [============= ] - 0s 193ms/step - loss: 0.0305 - acc: 0.9571 - val_loss: 0.1494 - val_ac
c: 0.7780
Epoch 96/200
1/1 [===========] - 0s 181ms/step - loss: 0.0309 - acc: 0.9429 - val_loss: 0.1496 - val_ac
c: 0.7820
Epoch 97/200
1/1 [============= ] - 0s 196ms/step - loss: 0.0291 - acc: 0.9857 - val_loss: 0.1513 - val_ac
c: 0.7800
Epoch 98/200
1/1 [============= ] - 0s 182ms/step - loss: 0.0317 - acc: 0.9643 - val_loss: 0.1525 - val_ac
c: 0.7780
Epoch 99/200
1/1 [=========== ] - 0s 189ms/step - loss: 0.0292 - acc: 0.9500 - val loss: 0.1520 - val ac
c: 0.7820
Epoch 100/200
c: 0.7780
Epoch 101/200
1/1 [============= ] - 0s 188ms/step - loss: 0.0312 - acc: 0.9643 - val_loss: 0.1515 - val_ac
c: 0.7760
Epoch 102/200
c: 0.7800
Epoch 103/200
c: 0.7840
Epoch 104/200
c: 0.7840
Epoch 105/200
1/1 [============= ] - 0s 188ms/step - loss: 0.0294 - acc: 0.9643 - val_loss: 0.1499 - val_ac
c: 0.7820
Epoch 106/200
1/1 [============ ] - 0s 185ms/step - loss: 0.0295 - acc: 0.9571 - val loss: 0.1486 - val ac
c: 0.7800
Epoch 107/200
c: 0.7840
Epoch 108/200
c: 0.7820
Epoch 109/200
c: 0.7880
Epoch 110/200
1/1 [=========== ] - 0s 191ms/step - loss: 0.0279 - acc: 0.9643 - val loss: 0.1469 - val ac
c: 0.7880
Epoch 111/200
c: 0.7860
Epoch 112/200
1/1 [===========] - 0s 199ms/step - loss: 0.0260 - acc: 0.9929 - val_loss: 0.1496 - val_ac
c: 0.7820
Epoch 113/200
c: 0.7780
Epoch 114/200
c: 0.7820
Epoch 115/200
c: 0.7800
Epoch 116/200
c: 0.7820
Epoch 117/200
c: 0.7780
Epoch 118/200
1/1 [==================] - 0s 187ms/step - loss: 0.0262 - acc: 0.9714 - val_loss: 0.1456 - val_ac
```

```
c: 0.7860
Epoch 119/200
c: 0.7820
Epoch 120/200
1/1 [============= ] - 0s 194ms/step - loss: 0.0277 - acc: 0.9429 - val_loss: 0.1462 - val_ac
c: 0.7820
Epoch 121/200
1/1 [===========] - 0s 203ms/step - loss: 0.0282 - acc: 0.9857 - val_loss: 0.1476 - val_ac
c: 0.7820
Epoch 122/200
c: 0.7840
Epoch 123/200
1/1 [============= ] - 0s 204ms/step - loss: 0.0269 - acc: 1.0000 - val_loss: 0.1516 - val_ac
c: 0.7780
Epoch 124/200
1/1 [============= ] - 0s 194ms/step - loss: 0.0260 - acc: 0.9714 - val_loss: 0.1535 - val_ac
c: 0.7740
Epoch 125/200
c: 0.7760
Epoch 126/200
c: 0.7800
Epoch 127/200
c: 0.7860
Epoch 128/200
c: 0.7800
Epoch 129/200
1/1 [=============== ] - 0s 260ms/step - loss: 0.0263 - acc: 0.9643 - val_loss: 0.1474 - val_ac
c: 0.7780
Epoch 130/200
c: 0.7800
Epoch 131/200
c: 0.7780
Epoch 132/200
c: 0.7740
Epoch 133/200
c: 0.7760
Epoch 134/200
1/1 [============= ] - 0s 195ms/step - loss: 0.0251 - acc: 0.9786 - val_loss: 0.1467 - val_ac
c: 0.7700
Epoch 135/200
c: 0.7720
Epoch 136/200
c: 0.7760
Epoch 137/200
1/1 [============= ] - 0s 218ms/step - loss: 0.0275 - acc: 0.9571 - val_loss: 0.1472 - val_ac
c: 0.7740
Epoch 138/200
c: 0.7680
Epoch 139/200
1/1 [=========== ] - 0s 192ms/step - loss: 0.0260 - acc: 0.9786 - val loss: 0.1464 - val ac
c: 0.7700
Epoch 140/200
c: 0.7680
Epoch 141/200
1/1 [============= ] - 0s 194ms/step - loss: 0.0242 - acc: 0.9786 - val_loss: 0.1451 - val_ac
c: 0.7720
Epoch 142/200
```

```
c: 0.7740
Epoch 143/200
1/1 [============= ] - 0s 183ms/step - loss: 0.0262 - acc: 0.9786 - val_loss: 0.1453 - val_ac
c: 0.7760
Epoch 144/200
c: 0.7840
Epoch 145/200
c: 0.7780
Epoch 146/200
1/1 [============= ] - 0s 188ms/step - loss: 0.0246 - acc: 0.9643 - val_loss: 0.1469 - val_ac
c: 0.7800
Epoch 147/200
1/1 [============= ] - 0s 182ms/step - loss: 0.0259 - acc: 0.9643 - val_loss: 0.1480 - val_ac
c: 0.7840
Epoch 148/200
1/1 [=========== ] - 0s 186ms/step - loss: 0.0256 - acc: 0.9571 - val loss: 0.1490 - val ac
c: 0.7820
Epoch 149/200
c: 0.7760
Fnoch 150/200
c: 0.7640
Epoch 151/200
c: 0.7660
Epoch 152/200
c: 0.7720
Epoch 153/200
c: 0.7740
Epoch 154/200
c: 0.7760
Epoch 155/200
c: 0.7840
Epoch 156/200
1/1 [============= ] - 0s 189ms/step - loss: 0.0246 - acc: 0.9786 - val_loss: 0.1395 - val_ac
c: 0.7860
Epoch 157/200
c: 0.7840
Epoch 158/200
c: 0.7860
Epoch 159/200
1/1 [============ ] - 0s 181ms/step - loss: 0.0253 - acc: 0.9857 - val loss: 0.1416 - val ac
c: 0.7800
Epoch 160/200
c: 0.7800
Epoch 161/200
1/1 [=========== ] - 0s 185ms/step - loss: 0.0234 - acc: 0.9929 - val loss: 0.1474 - val ac
c: 0.7820
Epoch 162/200
c: 0.7780
Epoch 163/200
1/1 [============= ] - 0s 209ms/step - loss: 0.0214 - acc: 0.9929 - val_loss: 0.1480 - val_ac
c: 0.7740
Epoch 164/200
1/1 [============== ] - 0s 195ms/step - loss: 0.0251 - acc: 0.9571 - val_loss: 0.1465 - val_ac
c: 0.7740
Epoch 165/200
1/1 [============] - 0s 187ms/step - loss: 0.0248 - acc: 0.9714 - val_loss: 0.1473 - val_ac
c: 0.7700
```

```
Epoch 166/200
1/1 [============= ] - 0s 195ms/step - loss: 0.0246 - acc: 0.9714 - val_loss: 0.1473 - val_ac
c: 0.7700
Epoch 167/200
1/1 [============] - 0s 188ms/step - loss: 0.0232 - acc: 0.9786 - val_loss: 0.1463 - val_ac
c: 0.7700
Epoch 168/200
1/1 [============= ] - 0s 188ms/step - loss: 0.0244 - acc: 0.9857 - val_loss: 0.1451 - val_ac
c: 0.7780
Epoch 169/200
1/1 [============= ] - 0s 200ms/step - loss: 0.0237 - acc: 0.9857 - val_loss: 0.1454 - val_ac
c: 0.7800
Epoch 170/200
1/1 [=========== ] - 0s 212ms/step - loss: 0.0273 - acc: 0.9429 - val loss: 0.1444 - val ac
c: 0.7860
Epoch 171/200
c: 0.7860
Epoch 172/200
1/1 [============= ] - 0s 193ms/step - loss: 0.0242 - acc: 0.9714 - val_loss: 0.1442 - val_ac
c: 0.7880
Epoch 173/200
c: 0.7880
Epoch 174/200
c: 0.7880
Epoch 175/200
c: 0.7840
Epoch 176/200
1/1 [============= ] - 0s 196ms/step - loss: 0.0237 - acc: 0.9643 - val_loss: 0.1489 - val_ac
c: 0.7740
Epoch 177/200
1/1 [=========== ] - 0s 184ms/step - loss: 0.0234 - acc: 0.9929 - val loss: 0.1509 - val ac
c: 0.7700
Epoch 178/200
c: 0.7660
Epoch 179/200
c: 0.7680
Epoch 180/200
c: 0.7740
Epoch 181/200
1/1 [=========== ] - 0s 203ms/step - loss: 0.0243 - acc: 0.9643 - val loss: 0.1448 - val ac
c: 0.7760
Epoch 182/200
c: 0.7760
Epoch 183/200
1/1 [============= ] - 0s 215ms/step - loss: 0.0227 - acc: 0.9714 - val_loss: 0.1428 - val_ac
c: 0.7780
Epoch 184/200
c: 0.7780
Epoch 185/200
c: 0.7780
Epoch 186/200
c: 0.7840
Epoch 187/200
c: 0.7840
Epoch 188/200
c: 0.7840
Epoch 189/200
1/1 [================] - 0s 300ms/step - loss: 0.0232 - acc: 0.9643 - val_loss: 0.1389 - val_ac
```

```
c: 0.7860
     Epoch 190/200
     c: 0.7920
     c: 0.8000
     Epoch 192/200
     1/1 [============ ] - 0s 190ms/step - loss: 0.0224 - acc: 0.9857 - val_loss: 0.1408 - val_ac
     c: 0.8000
     Epoch 193/200
     c: 0.7980
     Epoch 194/200
     1/1 [============= ] - 0s 176ms/step - loss: 0.0238 - acc: 0.9786 - val_loss: 0.1403 - val_ac
     c: 0.7960
     Epoch 195/200
     c: 0.7980
     Epoch 196/200
     c: 0.7940
     Epoch 197/200
     c: 0.7920
     Epoch 198/200
     1/1 [=============] - 0s 172ms/step - loss: 0.0247 - acc: 0.9714 - val_loss: 0.1426 - val_ac
     c: 0.7840
     Epoch 199/200
     1/1 [============= ] - 0s 179ms/step - loss: 0.0238 - acc: 0.9786 - val_loss: 0.1428 - val_ac
     c: 0.7820
     Epoch 200/200
     c: 0.7780
Out[ ]: <tensorflow.python.keras.callbacks.History at 0x1da4fbdeec8>
In [ ]: # 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))
     GCN Classification Report:
                     precision
                             recall f1-score support
            Case_Based
                       0.72
                             0.79
                                    0.75
                                           114
        Genetic_Algorithms
                       0.88
                             0.87
                                    0.87
                                           156
         Neural_Networks
                                    0.70
                       0.79
                             0.62
                                           290
      Probabilistic Methods
                       0.79
                             0.69
                                    0.74
                                           172
     Reinforcement_Learning
                       0.63
                             0.80
                                    0.70
                                           85
                             0.77
                                    0.62
           Rule_Learning
                       0.52
                                           60
               Theory
                       0.53
                             0.63
                                    0.58
                                           123
                                    0.72
                                          1000
              accuracy
                       0.69
                             0.74
                                    0.71
                                          1000
             macro avg
                       0.74
                             0.72
                                    0.72
                                          1000
           weighted avg
```

Get hidden layer representation for GCN

```
In []: 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])
```

```
In [ ]: 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)
          80 -
                                                                                                                   1
                                                                                                                   3
                                                                                                                   4
          60 -
                                                                                                                   5
          40
          20
           0
         -20
         -40
         -60
                      -60
                                     -40
                                                    -20
                                                                                   20
                                                                                                  40
                                                                                                                 60
```

Comparison to Fully-Connected Neural Networks

Building and Training FNN

```
In [ ]: es_patience = 100
    optimizer = Adam(lr=1e-2)
    12_reg = 5e-4
    epochs = 200
```

```
#Compare with FNN
#Construct the model
model_fnn = Sequential()
model_fnn.add(Dense(
                    input_dim=X.shape[1],
                    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
1/1 [==============] - 0s 279ms/step - loss: 0.2183 - acc: 0.1357 - val_loss: 0.4331 - val_ac
c: 0.2620
Epoch 2/200
n_batch_end) is slow compared to the batch update (0.155369). Check your callbacks.
c: 0.3780
Epoch 3/200
c: 0.5100
Epoch 4/200
1/1 [============= ] - 0s 175ms/step - loss: 0.1109 - acc: 0.7286 - val_loss: 0.3330 - val_ac
c: 0.5900
Epoch 5/200
1/1 [============ ] - 0s 240ms/step - loss: 0.0888 - acc: 0.7786 - val_loss: 0.2995 - val_ac
c: 0.5880
Epoch 6/200
1/1 [=========== ] - 0s 222ms/step - loss: 0.0647 - acc: 0.8429 - val loss: 0.2698 - val ac
c: 0.5980
Epoch 7/200
1/1 [==============] - 0s 285ms/step - loss: 0.0535 - acc: 0.9071 - val_loss: 0.2639 - val_ac
c: 0.5440
Fnoch 8/200
c: 0.5540
Epoch 9/200
c: 0.5580
Epoch 10/200
c: 0.5560
Epoch 11/200
c: 0.5640
Epoch 12/200
1/1 [============= ] - 0s 260ms/step - loss: 0.0412 - acc: 0.9929 - val_loss: 0.3126 - val_ac
c: 0.5700
Epoch 13/200
c: 0.5800
Epoch 14/200
1/1 [============= ] - 0s 257ms/step - loss: 0.0393 - acc: 0.9857 - val_loss: 0.3288 - val_ac
c: 0.5840
Epoch 15/200
c: 0.5780
Epoch 16/200
c: 0.5700
Epoch 17/200
1/1 [=========== ] - 0s 295ms/step - loss: 0.0314 - acc: 0.9857 - val loss: 0.3805 - val ac
c: 0.5720
Epoch 18/200
c: 0.5700
Epoch 19/200
1/1 [=========== ] - 1s 536ms/step - loss: 0.0280 - acc: 0.9786 - val loss: 0.3876 - val ac
c: 0.5620
Epoch 20/200
c: 0.5560
Epoch 21/200
1/1 [==========] - 1s 562ms/step - loss: 0.0235 - acc: 0.9929 - val_loss: 0.3967 - val_ac
c: 0.5380
Epoch 22/200
c: 0.5180
Epoch 23/200
1/1 [============] - 0s 273ms/step - loss: 0.0230 - acc: 0.9857 - val_loss: 0.4159 - val_ac
c: 0.5060
```

```
Epoch 24/200
c: 0.4880
Epoch 25/200
1/1 [===========] - 0s 313ms/step - loss: 0.0201 - acc: 0.9929 - val_loss: 0.3974 - val_ac
c: 0.5040
Epoch 26/200
1/1 [============= ] - 0s 346ms/step - loss: 0.0204 - acc: 0.9857 - val_loss: 0.3827 - val_ac
c: 0.5140
Epoch 27/200
1/1 [============= ] - 0s 284ms/step - loss: 0.0204 - acc: 0.9857 - val_loss: 0.3737 - val_ac
c: 0.5200
Epoch 28/200
1/1 [=========== ] - 0s 306ms/step - loss: 0.0198 - acc: 0.9786 - val loss: 0.3581 - val ac
c: 0.5200
Epoch 29/200
c: 0.5140
Epoch 30/200
1/1 [==========] - 0s 253ms/step - loss: 0.0184 - acc: 0.9929 - val_loss: 0.3600 - val_ac
c: 0.5120
Epoch 31/200
c: 0.5140
Epoch 32/200
c: 0.5060
Epoch 33/200
c: 0.5180
Epoch 34/200
1/1 [============= ] - 0s 246ms/step - loss: 0.0194 - acc: 0.9857 - val_loss: 0.3513 - val_ac
c: 0.5220
Epoch 35/200
c: 0.5300
Epoch 36/200
1/1 [============== ] - 0s 286ms/step - loss: 0.0186 - acc: 0.9929 - val_loss: 0.3340 - val_ac
c: 0.5260
Epoch 37/200
c: 0.5460
Epoch 38/200
c: 0.5460
Epoch 39/200
1/1 [=========== ] - 0s 246ms/step - loss: 0.0195 - acc: 0.9786 - val loss: 0.3276 - val ac
c: 0.5440
Epoch 40/200
c: 0.5540
Epoch 41/200
1/1 [============ ] - 0s 180ms/step - loss: 0.0190 - acc: 0.9929 - val_loss: 0.3387 - val_ac
c: 0.5420
Epoch 42/200
1/1 [=============== ] - 0s 191ms/step - loss: 0.0189 - acc: 0.9929 - val_loss: 0.3466 - val_ac
c: 0.5360
Epoch 43/200
c: 0.5240
Epoch 44/200
c: 0.5180
Epoch 45/200
c: 0.5180
Epoch 46/200
c: 0.5220
Epoch 47/200
1/1 [=================] - 0s 169ms/step - loss: 0.0178 - acc: 0.9929 - val_loss: 0.3731 - val_ac
```

```
c: 0.5200
Epoch 48/200
c: 0.5220
Epoch 49/200
1/1 [==========] - 0s 169ms/step - loss: 0.0162 - acc: 1.0000 - val_loss: 0.3664 - val_ac
c: 0.5280
Epoch 50/200
1/1 [===========] - 0s 172ms/step - loss: 0.0159 - acc: 1.0000 - val_loss: 0.3673 - val_ac
c: 0.5180
Epoch 51/200
c: 0.5140
Epoch 52/200
1/1 [============ ] - 0s 158ms/step - loss: 0.0155 - acc: 1.0000 - val_loss: 0.3745 - val_ac
c: 0.5120
Epoch 53/200
c: 0.5300
Epoch 54/200
c: 0.5180
Epoch 55/200
1/1 [=========== ] - 0s 166ms/step - loss: 0.0160 - acc: 0.9857 - val loss: 0.3840 - val ac
c: 0.5160
Epoch 56/200
c: 0.5060
Epoch 57/200
c: 0.5020
Epoch 58/200
c: 0.5060
Epoch 59/200
c: 0.5000
Epoch 60/200
c: 0.5060
Epoch 61/200
c: 0.5220
Epoch 62/200
c: 0.5280
Epoch 63/200
1/1 [============ ] - 0s 191ms/step - loss: 0.0173 - acc: 1.0000 - val_loss: 0.3396 - val_ac
c: 0.5240
Epoch 64/200
c: 0.5080
Epoch 65/200
1/1 [============== ] - 0s 200ms/step - loss: 0.0208 - acc: 0.9714 - val_loss: 0.4034 - val_ac
c: 0.4920
Epoch 66/200
1/1 [============= ] - 0s 193ms/step - loss: 0.0212 - acc: 0.9857 - val_loss: 0.4225 - val_ac
c: 0.4960
Epoch 67/200
c: 0.4940
Epoch 68/200
c: 0.4920
Epoch 69/200
c: 0.4880
Epoch 70/200
1/1 [============= ] - 0s 158ms/step - loss: 0.0265 - acc: 0.9786 - val_loss: 0.4416 - val_ac
c: 0.4860
Epoch 71/200
```

```
c: 0.4800
Epoch 72/200
c: 0.4780
Epoch 73/200
c: 0.4680
Epoch 74/200
c: 0.4700
Epoch 75/200
1/1 [============= ] - 0s 182ms/step - loss: 0.0240 - acc: 0.9786 - val_loss: 0.4211 - val_ac
c: 0.4840
Epoch 76/200
1/1 [============= ] - 0s 176ms/step - loss: 0.0287 - acc: 0.9643 - val_loss: 0.4028 - val_ac
c: 0.4800
Epoch 77/200
1/1 [=========== ] - 0s 215ms/step - loss: 0.0271 - acc: 0.9714 - val loss: 0.3904 - val ac
c: 0.4780
Epoch 78/200
1/1 [=============] - 0s 174ms/step - loss: 0.0237 - acc: 1.0000 - val_loss: 0.3874 - val_ac
c: 0.4840
Fnoch 79/200
c: 0.4820
Epoch 80/200
c: 0.4920
Epoch 81/200
c: 0.4960
Epoch 82/200
c: 0.4980
Epoch 83/200
1/1 [============= ] - 0s 171ms/step - loss: 0.0270 - acc: 0.9857 - val_loss: 0.3915 - val_ac
c: 0.5120
Epoch 84/200
c: 0.5160
Epoch 85/200
1/1 [============= ] - 0s 177ms/step - loss: 0.0273 - acc: 0.9714 - val_loss: 0.4138 - val_ac
c: 0.5080
Epoch 86/200
c: 0.5200
Epoch 87/200
c: 0.5240
Epoch 88/200
1/1 [=========== ] - 0s 200ms/step - loss: 0.0269 - acc: 0.9929 - val loss: 0.4038 - val ac
c: 0.5320
Epoch 89/200
c: 0.5240
Epoch 90/200
1/1 [=========== ] - 0s 206ms/step - loss: 0.0270 - acc: 0.9857 - val loss: 0.4036 - val ac
c: 0.5100
Epoch 91/200
c: 0.4980
Epoch 92/200
1/1 [============= ] - 0s 199ms/step - loss: 0.0274 - acc: 0.9714 - val_loss: 0.4255 - val_ac
c: 0.4900
Epoch 93/200
1/1 [============= ] - 0s 273ms/step - loss: 0.0260 - acc: 0.9857 - val_loss: 0.4271 - val_ac
c: 0.4840
Epoch 94/200
1/1 [===========] - 0s 199ms/step - loss: 0.0260 - acc: 0.9786 - val_loss: 0.4209 - val_ac
c: 0.4900
```

```
Epoch 95/200
    c: 0.4940
    Epoch 96/200
    c: 0.4780
    Epoch 97/200
    c: 0.4840
    Epoch 98/200
    c: 0.4760
    Epoch 99/200
    1/1 [=========== ] - 0s 196ms/step - loss: 0.0249 - acc: 0.9786 - val loss: 0.4278 - val ac
    c: 0.4640
    Epoch 100/200
    c: 0.4640
    Epoch 101/200
    1/1 [============= ] - 0s 206ms/step - loss: 0.0246 - acc: 0.9857 - val_loss: 0.4293 - val_ac
    c: 0.4580
    Epoch 102/200
    c: 0.4600
    Epoch 103/200
    c: 0.4580
    Epoch 104/200
    c: 0.4640
    Epoch 105/200
    c: 0.4720
    Epoch 106/200
    c: 0.4900
    Epoch 107/200
    1/1 [============== ] - 0s 174ms/step - loss: 0.0269 - acc: 0.9857 - val_loss: 0.3630 - val_ac
    c: 0.5120
Out[]: <tensorflow.python.keras.callbacks.History at 0x1da5dc56f88>
In [ ]: # 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:
                 precision
                        recall f1-score
                                  support
          Case_Based
                   0.63
                         0.48
                              0.55
                                    114
      Genetic_Algorithms
                   0.69
                         0.75
                              0.72
                                    156
        Neural Networks
                   0.73
                         0.46
                              0.56
                                    290
     Probabilistic_Methods
                   0.68
                         0.52
                              0.59
                                    172
                   0.32
                         0.56
                              0.41
                                    85
    Reinforcement_Learning
         Rule_Learning
                   0.46
                         0.57
                              0.51
                                    60
                              0.46
             Theory
                   0.36
                         0.62
                                    123
                              0.55
                                   1000
           accuracy
                   0.55
                         0.57
                              0.54
                                   1000
           macro avg
         weighted avg
                   0.61
                         0.55
                              0.56
                                   1000
```

Get hidden layer representation for FNN

```
In []: 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])
In []: x_tsne = TSNE(n_components=2).fit_transform(activations[3])
```

In []: ### END OF NOTEBOOK ###

