The codes are modified from the following source:\

1. https://github.com/bentrevett/pytorch-sentiment-analysis/blob/master/3%20-%20Faster%20Sentiment%20Analysis.ipynb
2. https://github.com/pyg-team/pytorch_geometric/blob/master/examples/node2vec.py
3. https://colab.research.google.com/drive/1h3-vJGRVloF5zStxL5l0rSy4ZUPNsjy8?usp=sharing#scrollTo=ci-LpZWhRJoI

Word Embedding

We will use word embedding to predict the sentiment of each sentence in IMDB data. Our plan is to use Keras to pre-process the data, and use Pytorch to build classification model and train the data.

Preparing Data

Keras provides us an easy and transparant way to process the data.

```
import numpy as np
import keras
import torch
import torch.nn as nn
import matplotlib.pyplot as plt
from keras.datasets import imdb
from torch.utils.data import Dataset, DataLoader
from pprint import pprint

np.set_printoptions(formatter={'float': lambda x: "{0:0.4f}".format(x)})
```

Next, let's load the training and test datasets.

To save training time, let's only keep the 10,000 most frequent words in the corpus. You can increase the number of words to get better performance

```
imdb = keras.datasets.imdb
num_words = 10000           # Only the 10,000 most frequent words

# Load data from keras
(train_data, train_labels), (test_data, test_labels) = imdb.load_data(seed=1, num_wo

# The first review of the data
print(train_data[0])
print(len(train_data[0]))
```

```
print('label:', train_labels[0])
```

```
Downloading data from https://storage.googleapis.com/tensorflow/tf-keras-datasets/imdb.
17465344/17464789 [==============================] - 0s 0us/step
17473536/17464789 [==============================] - 0s 0us/step
[1, 13, 28, 1039, 7, 14, 23, 1856, 13, 104, 36, 4, 699, 8060, 144, 297, 14, 175, 291, 1
284
label: 0
```

For processing raw text from the scratch, there are many tutorials online that you can follow. For example, here or here.

We see that the text of each review has been encoded as a sequence of integers. Each word in the text is represented as an integer. A dictionary called the `vocabulary` links each word to a unique integer. In the example above, we see that the integer 13 is repeated many times. This integer corresponds to a very frequent word 'i'. In fact, in the `vocabulary`, the more frequent a word, the lower the integer.

To get a fixed length input, we can simply truncate the documents to a fixed number of words, say 256. For documents that have more than 256 words, we will keep only the first 256 words. For shorter document, we will fill the unused word slots with zeros. However, you need to study the distribution of document lengths to ensure most documents are not truncated to maintain the content completeness.

With keras, this is easy to do:

```
train_data = keras.preprocessing.sequence.pad_sequences(train_data,
                                                        value=0,
                                                        padding='post',
                                                        maxlen=256)

test_data = keras.preprocessing.sequence.pad_sequences(test_data,
                                                       value=0,
                                                       padding='post',
                                                       maxlen=256)


# You can check one and notice 0s are appended at the end

train_data[1]
```

```
array([   1,  103,  450,  576,   73, 2896,    8,    4,  213,    7,  897,
         13,   16,  576, 3521,   19,    4,   22,    4,   22,   16,  465,
        728,    4, 2563,    4, 1460,    4, 3237,    5,    6,   55,  576,
       1078, 2734,   10,   10,   13,   69, 2721,  873,    8,   67,  111,
```

```
          318,  302,    5,   40,    6,    2,    2,   12, 4280,   72,  245,
           19,    4, 4211,    5,    4,    2,    7,   12, 1620,   13,  244,
          174, 2654,  245,   19,  129, 7102,   19,    4,  979,    7,    4,
           65,    5,  129,  459,    7,    4,  318,  302,   25,   80,  140,
            6,  196,   96,   61,  464,   13,   80,  407,   30,    4, 2217,
            7,  129,  337, 1333,   10,   10, 2127,    2,    4,  118,  284,
         1344,   16,    4,  612,   31, 1099,   25,   93, 1792, 7606,  168,
           40,    6,  506, 1079,    8,    2,   10,   10,  444,    4,  116,
           65,  347,    4,  312,  489, 1423,    5, 1190,  302,   12,   16,
          777,   13,   43,  657,   12,   71, 1207,   13,  244,  267,  930,
            8,    4,    2,   19,  576,  312, 1398,    0,    0,    0,    0,
            0,    0,    0,    0,    0,    0,    0,    0,    0,    0,    0,
            0,    0,    0,    0,    0,    0,    0,    0,    0,    0,    0,
            0,    0,    0,    0,    0,    0,    0,    0,    0,    0,    0,
            0,    0,    0,    0,    0,    0,    0,    0,    0,    0,    0,
            0,    0,    0,    0,    0,    0,    0,    0,    0,    0,    0,
            0,    0,    0,    0,    0,    0,    0,    0,    0,    0,    0,
            0,    0,    0,    0,    0,    0,    0,    0,    0,    0,    0,
            0,    0,    0,    0,    0,    0,    0,    0,    0,    0,    0,
            0,    0,    0], dtype=int32)
```

```
# show mapping between words and index
# dict(sorted(imdb.get_word_index().items(), key=lambda x:x[1]))
```

```
# Decode text

# word_index is a dictionary mapping words to an integer index
word_index = imdb.get_word_index()

# We reverse it, mapping integer indices to words
reverse_word_index = dict([(value, key) for (key, value) in word_index.items()])

# We decode the review; note that our indices were offset by 3
# because 0, 1 and 2 are reserved indices for "padding", "start of sequence", and "unknown".
decoded_review = ' '.join([reverse_word_index.get(i - 3, '?') for i in train_data[0]])

print(decoded_review)
```

```
Downloading data from https://storage.googleapis.com/tensorflow/tf-keras-datasets/imdb_
1646592/1641221 [==============================] - 0s 0us/step
1654784/1641221 [==============================] - 0s 0us/step
forget what was and that we remember not to do the same mistakes again like putting som
```

Train word vectors by Gensim

Check tutorial here: https://machinelearningmastery.com/develop-word-embeddings-python-gensim/

Use Pretrained Wordvector - GloVe

Rather than training our own word vectors from scratch, we will leverage on GloVe. Its authors have released four text files with word vectors trained on different massive web datasets. We will use the smallest file (“ glove.6B.zip”), which was trained on a corpus of 6 billion tokens and contains a vocabulary of 400 thousand tokens. It provides text-encoded vectors of various sizes: 50-dimensional, 100-dimensional, 200-dimensional, 300-dimensional. To save training time, We'll use the 50-dimension vectors. A higher dimension can give you better results.

```
# load Glove word vector
import torchtext

vector = torchtext.vocab.GloVe(name='6B', dim=50)

vector["city"]
```

```
.vector_cache/glove.6B.zip: 862MB [02:39, 5.39MB/s]
100%|██████████| 399999/400000 [00:09<00:00, 43817.03it/s]
tensor([ 0.4394,  0.4327, -0.3665,  0.2778,  0.0629, -0.8020, -0.9304,  0.0164,
        -0.5503, -0.1628, -0.4035, -1.3975,  0.3208, -0.8895, -0.1885,  0.1152,
         0.0453,  0.8300, -0.8759,  0.7765,  0.5595,  0.0747, -0.8467,  0.4098,
        -0.5977, -2.0620, -0.1589,  0.5798,  0.2827, -1.0213,  3.2488,  0.5003,
         0.1156, -1.1707,  0.1902,  0.3689, -0.0420,  0.0282,  0.5412,  0.8489,
        -0.6671,  0.6080,  0.2379, -0.6538, -0.7055,  0.5165, -1.0780, -0.7152,
         0.4840, -0.3256])
```

Embedding matrix

Next we need to look up the Glove vector for each word used in our dataset.

We limit our vocabulary to 10,000 words.

Note, the first three words are reserved for padding, unknown tokens, and a symbol to indicate the start of a sentence. We use all zero vectors to represent these words.

```
# Look up word vector for each word in our vocabulary

vocab_size = 10000
emb_dim = 50
missing_words = []  # check if any word without a vector

# initialize embedding matrix
emb_weight = np.zeros((vocab_size, emb_dim))
```

```
# loop through all words
for word, idx in word_index.items():

  # align with word index in sentences, since the first 3 indexes are reserved
  if idx + 3 < vocab_size :
    try:
      emb = vector[word]
      emb_weight[idx+3] = emb

    # not every word has a vector
    except:
      missing_words.append(word)

print(missing_words)
```

```
[]
```

Check embeddings for a few words to ensure our embedding matrix is correct.

```
# get index for word city
i = word_index['city']

# remember to add 3 to the index
print(emb_weight[i+3])

# vector from Glove
vector["city"]
```

```
[0.4394 0.4327 -0.3665 0.2778 0.0629 -0.8020 -0.9304 0.0164 -0.5503
 -0.1628 -0.4035 -1.3975 0.3208 -0.8895 -0.1885 0.1152 0.0453 0.8300
 -0.8759 0.7765 0.5595 0.0747 -0.8467 0.4098 -0.5977 -2.0620 -0.1589
 0.5798 0.2827 -1.0213 3.2488 0.5003 0.1156 -1.1707 0.1902 0.3689 -0.0420
 0.0282 0.5412 0.8489 -0.6671 0.6080 0.2379 -0.6538 -0.7055 0.5165 -1.0780
 -0.7152 0.4840 -0.3256]
tensor([ 0.4394,  0.4327, -0.3665,  0.2778,  0.0629, -0.8020, -0.9304,  0.0164,
        -0.5503, -0.1628, -0.4035, -1.3975,  0.3208, -0.8895, -0.1885,  0.1152,
         0.0453,  0.8300, -0.8759,  0.7765,  0.5595,  0.0747, -0.8467,  0.4098,
        -0.5977, -2.0620, -0.1589,  0.5798,  0.2827, -1.0213,  3.2488,  0.5003,
         0.1156, -1.1707,  0.1902,  0.3689, -0.0420,  0.0282,  0.5412,  0.8489,
        -0.6671,  0.6080,  0.2379, -0.6538, -0.7055,  0.5165, -1.0780, -0.7152,
         0.4840, -0.3256])
```

Build the Model

The next stage is building the model that we'll eventually train and evaluate. We will build a simple model of 3 layers: the `embedding` layer, an average laery, and the linear layer:

- **Embedding layer**: look up for each word in the `emb_matrix` and convert a document to a matrix of shape `(doc_len, emb_dim)`. Here we use pretrained Glove vectors. We freeze `emb_matrix` to make it non-trainable. You can also continue to fine tune the vectors.

- **Average layer**: take the average of word vectors across all words in a document to create a representation for the document.
- **Linear layer**: produce the final prediction.

We now create a neural network with an embedding layer as first layer (we load into it the weights matrix).

```
import torch
import torch.nn as nn
import torch.nn.functional as F

class EmbNN(nn.Module):
    def __init__(self, emb_weight, emb_dim, output_dim):

        super().__init__()

        # Create a embedding layer using emb_weight.
        # Weights can be frozen or trainable
        self.embedding = nn.Embedding.from_pretrained(emb_weight, freeze=True)

        self.fc = nn.Linear(emb_dim, output_dim)

    def forward(self, text):

        #text shape: [batch size, sent len]

        embedded = self.embedding(text)
        #embedded shape: [batch size, sent len, emb dim]

        # Take average of word vectors in a sentence as the feature
        avg = embedded.mean(dim = 1)
        #avg shape: [batch size, emb_dim]

        output =  self.fc(avg)
        #output shape: [batch size, output_dim]

        return output


# create a model
output_dim = 1

emb_dim = 50

# convert emb_matrix to tensor
emb_matrix = torch.Tensor(emb_weight)
print(emb_matrix.shape)
```

```
model = EmbNN(emb_matrix,emb_dim, output_dim)
```

```
torch.Size([10000, 50])
```

Train the Model

Double-click (or enter) to edit

As usual, we first define train/test datasets.

```
class IMDB_dataset(Dataset):
    def __init__(self, x, y):
        self.x = torch.Tensor(x).long()
        self.y = torch.Tensor(y).float()

    def __getitem__(self, index):
        return self.x[index], self.y[index]

    def __len__(self):
        return self.x.size()[0]

# dataset
train_dataset = IMDB_dataset(train_data, train_labels)
test_dataset = IMDB_dataset(test_data, test_labels)
```

```
import torch.optim as optim

device = 'cuda' if torch.cuda.is_available() else 'cpu'
device
```

```
'cuda'
```

```
# the train function is reused from last lab

def train_model(model, train_dataset, test_dataset, device, lr=0.0001, epochs=20, batch_size=
    # construct dataloader
    train_loader = DataLoader(train_dataset, batch_size=batch_size, shuffle = True)
    test_loader = DataLoader(test_dataset, batch_size=batch_size)

    # move model to device
    model = model.to(device)

    # history
    history = {'train_loss': [],
               'train_acc': [],
```

```
            'test_loss': [],
            'test_acc': []}

    # setup loss function and optimizer
    criterion = nn.BCEWithLogitsLoss()
    optimizer = torch.optim.RMSprop(model.parameters(), lr=lr)

    # training loop
    print('Training Start')
    for epoch in range(epochs):
        model.train()
        train_loss = 0
        train_acc = 0
        test_loss = 0
        test_acc = 0
        for x, y in train_loader:
            # move data to device
            x = x.to(device)
            y = y.to(device)
            # forward
            outputs = model(x).view(-1) # (num_batch, 1) -> (num_batch,)
            pred = torch.round(torch.sigmoid(outputs))
            cur_train_loss = criterion(outputs, y)
            cur_train_acc = (pred == y).float().mean().item()
            # backward
            cur_train_loss.backward()
            optimizer.step()
            optimizer.zero_grad()
            # loss and acc
            train_loss += cur_train_loss
            train_acc += cur_train_acc

        # test start
        model.eval()
        with torch.no_grad():
            for x, y in test_loader:
                # move
                x = x.to(device)
                y = y.to(device)
                # predict
                outputs = model(x).view(-1)
                pred = torch.round(torch.sigmoid(outputs))
                cur_test_loss = criterion(outputs, y)
                cur_test_acc = (pred == y).float().mean().item()
                # loss and acc
                test_loss += cur_test_loss
                test_acc += cur_test_acc

        # epoch output
        train_loss = (train_loss/len(train_loader)).item()
        train_acc = train_acc/len(train_loader)
```

```
        val_loss = (test_loss/len(test_loader)).item()
        val_acc = test_acc/len(test_loader)
        history['train_loss'].append(train_loss)
        history['train_acc'].append(train_acc)
        history['test_loss'].append(val_loss)
        history['test_acc'].append(val_acc)
        print(f"Epoch:{epoch + 1} / {epochs}, train loss:{train_loss:.3f} train_acc:{train_ac

    return history

hist = train_model(model, train_dataset, test_dataset, device, \
                   lr=0.0005, epochs = 50, batch_size = 64)
```

```
Training Start
Epoch:1 / 50, train loss:0.686 train_acc:0.584, validation loss:0.681 validation acc:0.
Epoch:2 / 50, train loss:0.675 train_acc:0.636, validation loss:0.672 validation acc:0.
Epoch:3 / 50, train loss:0.667 train_acc:0.654, validation loss:0.664 validation acc:0.
Epoch:4 / 50, train loss:0.659 train_acc:0.662, validation loss:0.658 validation acc:0.
Epoch:5 / 50, train loss:0.653 train_acc:0.667, validation loss:0.652 validation acc:0.
Epoch:6 / 50, train loss:0.647 train_acc:0.670, validation loss:0.647 validation acc:0.
Epoch:7 / 50, train loss:0.641 train_acc:0.675, validation loss:0.642 validation acc:0.
Epoch:8 / 50, train loss:0.636 train_acc:0.676, validation loss:0.637 validation acc:0.
Epoch:9 / 50, train loss:0.631 train_acc:0.680, validation loss:0.633 validation acc:0.
Epoch:10 / 50, train loss:0.627 train_acc:0.683, validation loss:0.629 validation acc:0
Epoch:11 / 50, train loss:0.623 train_acc:0.685, validation loss:0.626 validation acc:0
Epoch:12 / 50, train loss:0.620 train_acc:0.688, validation loss:0.623 validation acc:0
Epoch:13 / 50, train loss:0.617 train_acc:0.690, validation loss:0.620 validation acc:0
Epoch:14 / 50, train loss:0.613 train_acc:0.692, validation loss:0.617 validation acc:0
Epoch:15 / 50, train loss:0.611 train_acc:0.694, validation loss:0.614 validation acc:0
Epoch:16 / 50, train loss:0.608 train_acc:0.697, validation loss:0.612 validation acc:0
Epoch:17 / 50, train loss:0.605 train_acc:0.698, validation loss:0.609 validation acc:0
Epoch:18 / 50, train loss:0.603 train_acc:0.700, validation loss:0.607 validation acc:0
Epoch:19 / 50, train loss:0.600 train_acc:0.701, validation loss:0.604 validation acc:0
Epoch:20 / 50, train loss:0.598 train_acc:0.703, validation loss:0.602 validation acc:0
Epoch:21 / 50, train loss:0.596 train_acc:0.706, validation loss:0.600 validation acc:0
Epoch:22 / 50, train loss:0.594 train_acc:0.707, validation loss:0.598 validation acc:0
Epoch:23 / 50, train loss:0.592 train_acc:0.708, validation loss:0.596 validation acc:0
Epoch:24 / 50, train loss:0.590 train_acc:0.709, validation loss:0.595 validation acc:0
Epoch:25 / 50, train loss:0.588 train_acc:0.711, validation loss:0.593 validation acc:0
Epoch:26 / 50, train loss:0.586 train_acc:0.711, validation loss:0.591 validation acc:0
Epoch:27 / 50, train loss:0.585 train_acc:0.713, validation loss:0.590 validation acc:0
Epoch:28 / 50, train loss:0.583 train_acc:0.713, validation loss:0.588 validation acc:0
Epoch:29 / 50, train loss:0.582 train_acc:0.715, validation loss:0.587 validation acc:0
Epoch:30 / 50, train loss:0.580 train_acc:0.716, validation loss:0.585 validation acc:0
Epoch:31 / 50, train loss:0.579 train_acc:0.717, validation loss:0.584 validation acc:0
Epoch:32 / 50, train loss:0.577 train_acc:0.719, validation loss:0.583 validation acc:0
Epoch:33 / 50, train loss:0.576 train_acc:0.719, validation loss:0.581 validation acc:0
Epoch:34 / 50, train loss:0.575 train_acc:0.721, validation loss:0.580 validation acc:0
Epoch:35 / 50, train loss:0.574 train_acc:0.721, validation loss:0.579 validation acc:0
Epoch:36 / 50, train loss:0.572 train_acc:0.722, validation loss:0.578 validation acc:0
Epoch:37 / 50, train loss:0.571 train_acc:0.722, validation loss:0.577 validation acc:0
Epoch:38 / 50, train loss:0.570 train_acc:0.724, validation loss:0.576 validation acc:0
Epoch:39 / 50, train loss:0.569 train_acc:0.724, validation loss:0.575 validation acc:0
Epoch:40 / 50, train loss:0.568 train_acc:0.726, validation loss:0.574 validation acc:0
Epoch:41 / 50, train loss:0.567 train_acc:0.726, validation loss:0.573 validation acc:0
```

```
Epoch:42 / 50, train loss:0.566 train_acc:0.726, validation loss:0.572 validation acc:0
Epoch:43 / 50, train loss:0.565 train_acc:0.727, validation loss:0.571 validation acc:0
Epoch:44 / 50, train loss:0.564 train_acc:0.728, validation loss:0.570 validation acc:0
Epoch:45 / 50, train loss:0.564 train_acc:0.728, validation loss:0.569 validation acc:0
Epoch:46 / 50, train loss:0.563 train_acc:0.728, validation loss:0.569 validation acc:0
Epoch:47 / 50, train loss:0.562 train_acc:0.729, validation loss:0.568 validation acc:0
Epoch:48 / 50, train loss:0.561 train_acc:0.728, validation loss:0.567 validation acc:0
Epoch:49 / 50, train loss:0.560 train_acc:0.731, validation loss:0.566 validation acc:0
Epoch:50 / 50, train loss:0.560 train_acc:0.731, validation loss:0.566 validation acc:0
```

Node2Vec Embedding Example

We will use the well-known network of Zachary's karate club to illustrate Node2Vec method. This graph describes a social network of 34 members of a karate club and documents links between members.

```
import torch

print(torch.__version__)
```

```
1.10.0+cu111
```

We'll use package `node2vec`. This package is a Python implementation of the node2vec algorithm. Given any graph, it can learn continuous feature representations for the nodes, which can then be used for various downstream machine learning tasks. You can find more details about the package here.

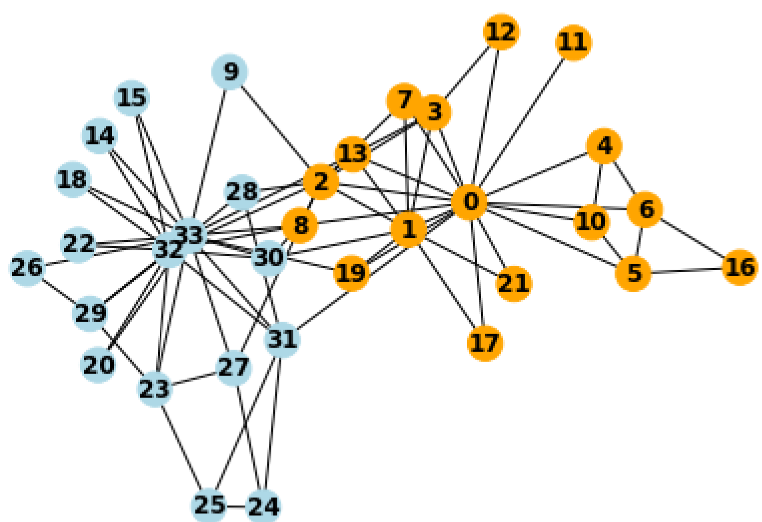
```
!pip install node2vec
```

```
Collecting node2vec
  Downloading node2vec-0.4.3.tar.gz (4.6 kB)
Requirement already satisfied: networkx in /usr/local/lib/python3.7/dist-packages (from
Requirement already satisfied: gensim in /usr/local/lib/python3.7/dist-packages (from n
Requirement already satisfied: numpy in /usr/local/lib/python3.7/dist-packages (from no
Requirement already satisfied: tqdm in /usr/local/lib/python3.7/dist-packages (from nod
Requirement already satisfied: joblib>=0.13.2 in /usr/local/lib/python3.7/dist-packages
Requirement already satisfied: six>=1.5.0 in /usr/local/lib/python3.7/dist-packages (fr
Requirement already satisfied: smart-open>=1.2.1 in /usr/local/lib/python3.7/dist-packa
Requirement already satisfied: scipy>=0.18.1 in /usr/local/lib/python3.7/dist-packages
Building wheels for collected packages: node2vec
  Building wheel for node2vec (setup.py) ... done
  Created wheel for node2vec: filename=node2vec-0.4.3-py3-none-any.whl size=5980 sha256
  Stored in directory: /root/.cache/pip/wheels/07/62/78/5202cb8c03cbf1593b48a8a442fca8c
Successfully built node2vec
Installing collected packages: node2vec
Successfully installed node2vec-0.4.3
```

Visualize Graph

```
import networkx as nx


# Load the Zachary's Karate Club as a NetworkX Graph object
KCG = nx.karate_club_graph()

# each node has a class, either "Mr. Hi" or "Officer"
labels = [KCG.nodes[i]['club'] for i in KCG.nodes]
print(labels)

color_map = ['lightblue' if l == 'Officer' else 'orange' for l in labels]

nx.draw(KCG, with_labels=True, font_weight='bold', \
        node_color=color_map)
```

```
['Mr. Hi', 'Mr. Hi', 'Mr. Hi', 'Mr. Hi', 'Mr. Hi', 'Mr. Hi', 'Mr. Hi', 'Mr. Hi', '
```

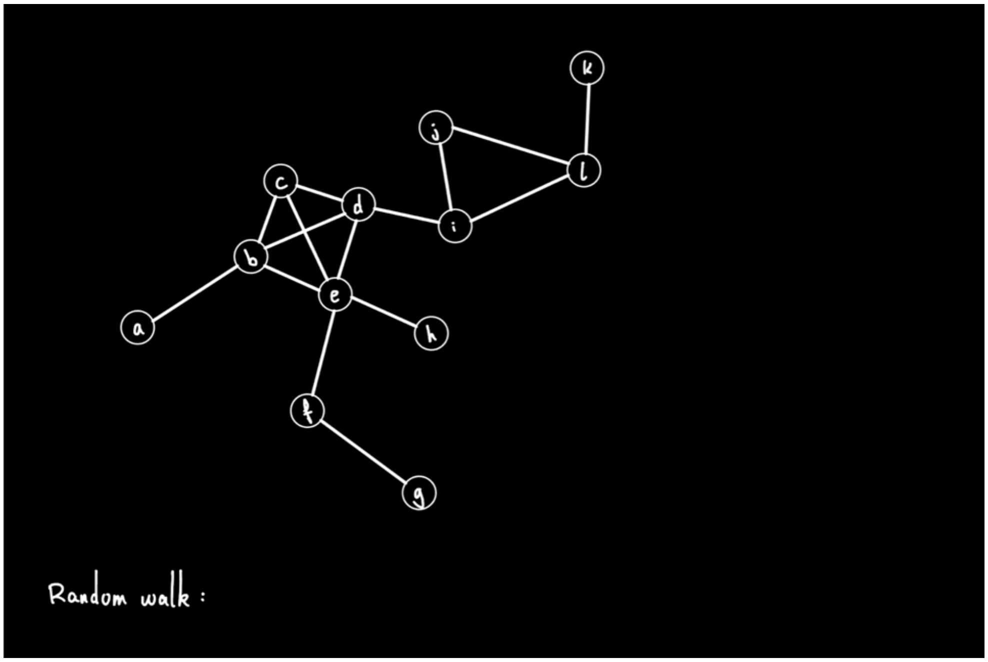


After initializing the KarateClub dataset, we first can inspect some of its properties. This graph has 34 nodes, and 156 undirected edges. Nodes belong two classes: 'Officer' or 'Mr. Hi'. Each edge stands for communication between two nodes.

Random Walk

Firstly, we will learn to do the node embedding. There are different embedding generation methods like node2vec, DeepWalk etc. In this example, we will use node2vec.

Animation of random walk



(References: https://towardsdatascience.com/node2vec-explained-graphically-749e49b7eb6b)

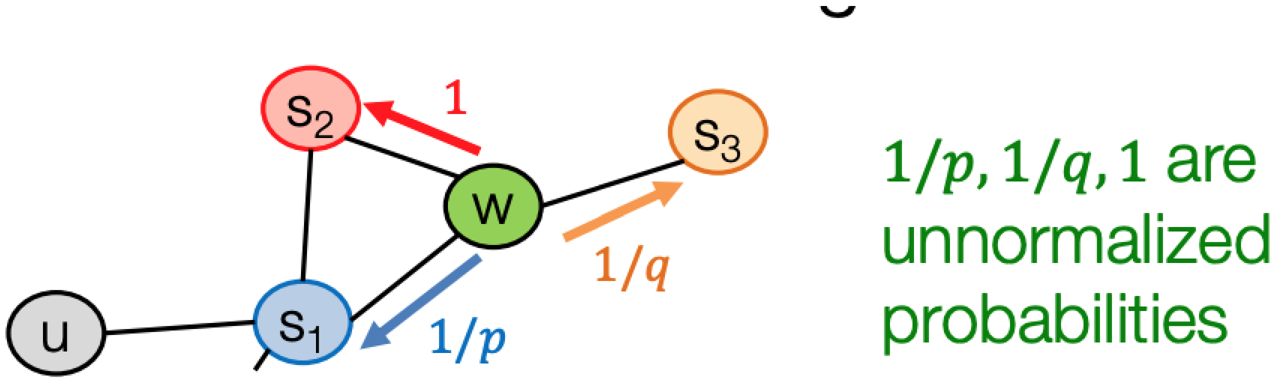
```
from node2vec import Node2Vec
# generate walks
node2vec = Node2Vec(KCG, dimensions=64, walk_length=10,num_walks=80)    # walk_length: How ma
#Embed nodes                                                                              # nu
node2vec_model = node2vec.fit(window=10, min_count=1,batch_words=4)                       # p:
                                                                                          # q:
# get embeddings
# The variable embeddings stores the embeddings in form of a dictionary where the keys are th
embeddings_map = node2vec_model.wv
embeddings = embeddings_map[[str(i) for i in range(len(KCG.nodes))]]

embeddings.shape
#Note: any keywords acceptable by gensim.Word2vec can be passed
```

Computing transition probabilities: 100% 34/34 [00:00<00:00, 527.15it/s]

```
Generating walks (CPU: 1): 100%|██████████| 80/80 [00:01<00:00, 41.94it/s]
(34, 64)
```

Biased Walk

We can set biased walking policy by adjusting parameters `p` and `q` in 'Node2Vec'




```
# p: controls the probability to go back
# q: controls the probability to explore

Node2Vec(KCG, dimensions=64, walk_length=10,num_walks=80, workers=1,p=1,q=2)
Node2Vec(KCG, dimensions=64, walk_length=10,num_walks=80, workers=1,p=2,q=1)
```

```
Computing transition probabilities: 100%  34/34 [00:00<00:00, 895.54it/s]
Generating walks (CPU: 1): 100%|██████████| 80/80 [00:01<00:00, 76.97it/s]
Computing transition probabilities: 100%  34/34 [00:00<00:00, 724.66it/s]
```

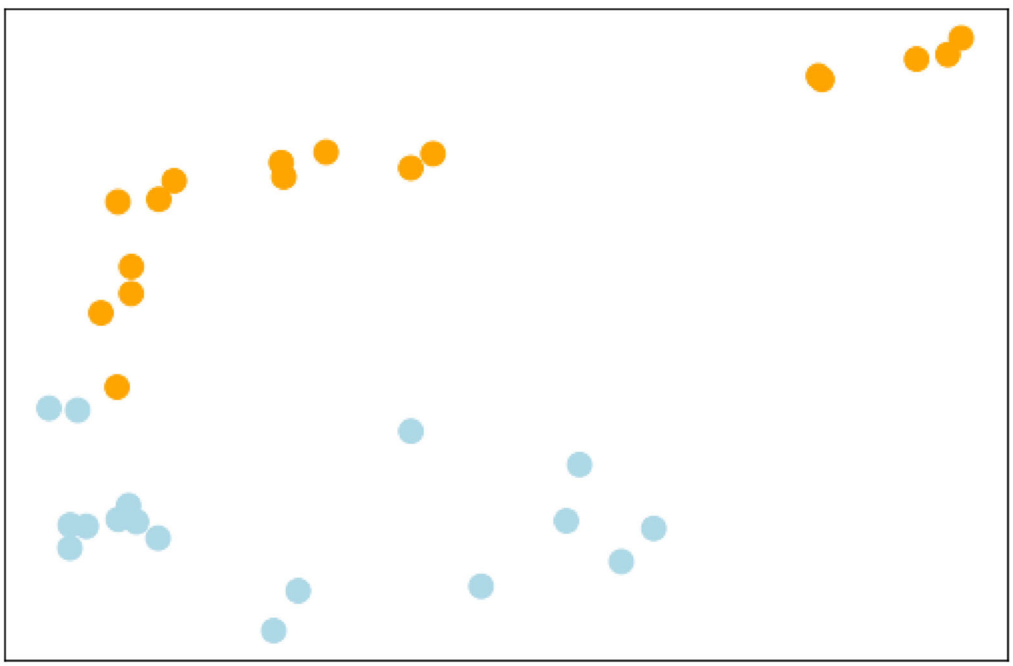
Visualize the embeddings

Embeddings are just low-dimensional numerical representations of the network, therefore we can make a visualization of these embeddings. Here, the size of the embeddings is 64, so we need to employ t-SNE which is a dimensionality reduction technique. Basically, t-SNE transforms the 64 dimension array into a 2-dimensional array so that we can visualize it in a 2D space. We can observe the 4groups of nodes are separated decently in the 2D space. The node embeddings are informative.

```
#Visualize the embeddings
import numpy as np
from sklearn.manifold import TSNE
import matplotlib.pyplot as plt

# transform the embeddings from 64 dimensions to 2D space
# TSNE is a dimension deduction technique
m = TSNE(learning_rate=20, random_state=42)
```

```
tsne_features = m.fit_transform(list(embeddings))

# retrieve the labels for each node
#labels = data.y

# plot the transformed embeddings
plt.figure(figsize=(9,6))
plt.scatter(x = tsne_features[:,0],
            y = tsne_features[:,1],
            c = color_map,
            s =140,
            cmap="Set2",
            )
plt.xticks([])
plt.yticks([])
```

```
/usr/local/lib/python3.7/dist-packages/sklearn/manifold/_t_sne.py:783: FutureWarni
  FutureWarning,
([], <a list of 0 Text major ticklabel objects>)
```



Graph Neural Network (GNN)

References: https://towardsdatascience.com/a-beginners-guide-to-graph-neural-networks-using-pytorch-geometric-part-1-d98dc93e7742

Next, we use GNN to derive node representation and classify nodes into labels.

We divide the graph into train and test sets where we use the train set to build a graph neural network model and use the model to predict the missing node labels in the test set.

Here, we use PyTorch Geometric (PyG) python library to model the graph neural network. Alternatively, Deep Graph Library (DGL) can also be used for the same purpose. PyTorch Geometric is a geometric deep learning library built on top of PyTorch. Several popular graph neural network methods have been implemented using PyG and you can play around with the code using built-in datasets or create your own dataset. PyG uses a nifty implementation where it provides an InMemoryDataset class which can be used to create the custom dataset (Note: InMemoryDataset

Fist, install packages

```
import torch

!pip uninstall torch-scatter torch-sparse torch-geometric torch-cluster  --y
!pip install torch-scatter -f https://data.pyg.org/whl/torch-{torch.__version__}.html
!pip install torch-sparse -f https://data.pyg.org/whl/torch-{torch.__version__}.html
!pip install torch-cluster -f https://data.pyg.org/whl/torch-{torch.__version__}.html
!pip install git+https://github.com/pyg-team/pytorch_geometric.git
```

```
WARNING: Skipping torch-scatter as it is not installed.
WARNING: Skipping torch-sparse as it is not installed.
Found existing installation: torch-geometric 2.1.0.post1
Uninstalling torch-geometric-2.1.0.post1:
  Successfully uninstalled torch-geometric-2.1.0.post1
WARNING: Skipping torch-cluster as it is not installed.
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/pub
Looking in links: https://data.pyg.org/whl/torch-1.12.1+cu113.html
Collecting torch-scatter
  Downloading https://data.pyg.org/whl/torch-1.12.0%2Bcu113/torch_scatter-2.0.9-cp37-cp
     |████████████████████████████████| 7.9 MB 2.8 MB/s
Installing collected packages: torch-scatter
Successfully installed torch-scatter-2.0.9
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/pub
Looking in links: https://data.pyg.org/whl/torch-1.12.1+cu113.html
Collecting torch-sparse
  Downloading https://data.pyg.org/whl/torch-1.12.0%2Bcu113/torch_sparse-0.6.15-cp37-cp
     |████████████████████████████████| 3.5 MB 2.7 MB/s
Requirement already satisfied: scipy in /usr/local/lib/python3.7/dist-packages (from to
Requirement already satisfied: numpy<1.23.0,>=1.16.5 in /usr/local/lib/python3.7/dist-p
Installing collected packages: torch-sparse
Successfully installed torch-sparse-0.6.15
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/pub
Looking in links: https://data.pyg.org/whl/torch-1.12.1+cu113.html
Collecting torch-cluster
  Downloading https://data.pyg.org/whl/torch-1.12.0%2Bcu113/torch_cluster-1.6.0-cp37-cp
     |████████████████████████████████| 2.4 MB 2.0 MB/s
Installing collected packages: torch-cluster
Successfully installed torch-cluster-1.6.0
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-wheels/pub
Collecting git+https://github.com/pyg-team/pytorch_geometric.git
```

```
  Cloning https://github.com/pyg-team/pytorch_geometric.git to /tmp/pip-req-build-f5rrr
  Running command git clone -q https://github.com/pyg-team/pytorch_geometric.git /tmp/p
Requirement already satisfied: tqdm in /usr/local/lib/python3.7/dist-packages (from tor
Requirement already satisfied: numpy in /usr/local/lib/python3.7/dist-packages (from to
Requirement already satisfied: scipy in /usr/local/lib/python3.7/dist-packages (from to
Requirement already satisfied: jinja2 in /usr/local/lib/python3.7/dist-packages (from t
Requirement already satisfied: requests in /usr/local/lib/python3.7/dist-packages (from
Requirement already satisfied: pyparsing in /usr/local/lib/python3.7/dist-packages (fro
Requirement already satisfied: scikit-learn in /usr/local/lib/python3.7/dist-packages (
Requirement already satisfied: MarkupSafe>=0.23 in /usr/local/lib/python3.7/dist-packag
Requirement already satisfied: chardet<4,>=3.0.2 in /usr/local/lib/python3.7/dist-packa
Requirement already satisfied: idna<3,>=2.5 in /usr/local/lib/python3.7/dist-packages (
Requirement already satisfied: urllib3!=1.25.0,!=1.25.1,<1.26,>=1.21.1 in /usr/local/li
Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.7/dist-pack
Requirement already satisfied: joblib>=0.11 in /usr/local/lib/python3.7/dist-packages (
Requirement already satisfied: threadpoolctl>=2.0.0 in /usr/local/lib/python3.7/dist-pa
Building wheels for collected packages: torch-geometric
  Building wheel for torch-geometric (setup.py) ... done
  Created wheel for torch-geometric: filename=torch_geometric-2.1.0-py3-none-any.whl si
  Stored in directory: /tmp/pip-ephem-wheel-cache-359njut3/wheels/85/c9/07/7936efecad79
Successfully built torch-geometric
Installing collected packages: torch-geometric
Successfully installed torch-geometric-2.1.0
```

Prepare data

The karate club dataset can be loaded directly from the NetworkX library. We retrieve the labels from the graph and create an edge index in the coordinate format. The node degree was used as embeddings/ numerical representations for the nodes (In the case of a directed graph, in-degree can be used for the same purpose). Since degree values tend to be diverse, we normalize them before using the values as input to the GNN model.

```
import networkx as nx
import numpy as np
import torch
from sklearn.preprocessing import StandardScaler

# load graph from networkx library
G = nx.karate_club_graph()

# retrieve the labels for each node
labels = np.asarray([G.nodes[i]['club'] != 'Mr. Hi' for i in G.nodes]).astype(np.int64)

# create edge index from
adj = nx.to_scipy_sparse_matrix(G).tocoo()
row = torch.from_numpy(adj.row.astype(np.int64)).to(torch.long)
col = torch.from_numpy(adj.col.astype(np.int64)).to(torch.long)
```

```
edge_index = torch.stack([row, col], dim=0)

# using degree as embedding
embeddings = np.array(list(dict(G.degree()).values()))

# normalizing degree values
scale = StandardScaler()
embeddings = scale.fit_transform(embeddings.reshape(-1,1))
```

Split nodes into train/test via masking

The KarateDataset class inherits from the InMemoryDataset class and use a Data object to collate all information relating to the karate club dataset. The graph data is then split into train and test sets, thereby creating the train and test masks using the splits.

```
import torch
import pandas as pd
from torch_geometric.data import InMemoryDataset, Data
from sklearn.model_selection import train_test_split
import torch_geometric.transforms as T

# custom dataset
class KarateDataset(InMemoryDataset):
    def __init__(self, transform=None):
        super(KarateDataset, self).__init__('.', transform, None, None)

        data = Data(edge_index=edge_index)

        data.num_nodes = G.number_of_nodes()

        # embedding
        data.x = torch.from_numpy(embeddings).type(torch.float32)

        # labels
        y = torch.from_numpy(labels).type(torch.long)
        data.y = y.clone().detach()

        data.num_classes = 2

        # splitting the data into train, validation and test
        X_train, X_test, y_train, y_test = train_test_split(pd.Series(list(G.nodes())),
                                                            pd.Series(labels),
                                                            test_size=0.30,
                                                            random_state=42)

        n_nodes = G.number_of_nodes()
```

```
        # create train and test masks for data
        train_mask = torch.zeros(n_nodes, dtype=torch.bool)
        test_mask = torch.zeros(n_nodes, dtype=torch.bool)
        train_mask[X_train.index] = True
        test_mask[X_test.index] = True
        data['train_mask'] = train_mask
        data['test_mask'] = test_mask

        self.data, self.slices = self.collate([data])

    def _download(self):
        return

    def _process(self):
        return

    def __repr__(self):
        return '{}()'.format(self.__class__.__name__)

dataset = KarateDataset()
data = dataset[0]
```

Create GNN model (two-layer GNN)

```
import torch.nn as nn
import torch.nn.functional as F
from torch_geometric.nn import GCNConv

# GCN model with 2 layers
class Net(torch.nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.conv1 = GCNConv(data.num_features, 16)
        self.conv2 = GCNConv(16, int(data.num_classes))

    def forward(self):
        x, edge_index = data.x, data.edge_index
        x = F.relu(self.conv1(x, edge_index))
        x = F.dropout(x, training=self.training)
        x = self.conv2(x, edge_index)
        return F.log_softmax(x, dim=1)  # loss is calculated here

device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')

data =  data.to(device)

model = Net().to(device)
```

Train model

Pay extra attention to how the loss is calculated through masking

```
torch.manual_seed(42)

optimizer_name = "Adam"
lr = 1e-1
optimizer = getattr(torch.optim, optimizer_name)(model.parameters(), lr=lr)
epochs = 200

def train():
  model.train()
  optimizer.zero_grad()
  F.nll_loss(model()[data.train_mask], data.y[data.train_mask]).backward()
  optimizer.step()

@torch.no_grad()
def test():
  model.eval()
  logits = model()
  mask1 = data['train_mask']
  pred1 = logits[mask1].max(1)[1]
  acc1 = pred1.eq(data.y[mask1]).sum().item() / mask1.sum().item()
  mask = data['test_mask']
  pred = logits[mask].max(1)[1]
  acc = pred.eq(data.y[mask]).sum().item() / mask.sum().item()
  return acc1,acc

for epoch in range(1, epochs):
  train()

train_acc,test_acc = test()

print('#' * 70)
print('Train Accuracy: %s' %train_acc )
print('Test Accuracy: %s' % test_acc)
print('#' * 70)
```

```
######################################################################
Train Accuracy: 0.8695652173913043
Test Accuracy: 0.7272727272727273
######################################################################
```

New Section