Understanding Graph Convolutional Networks for Node Classification

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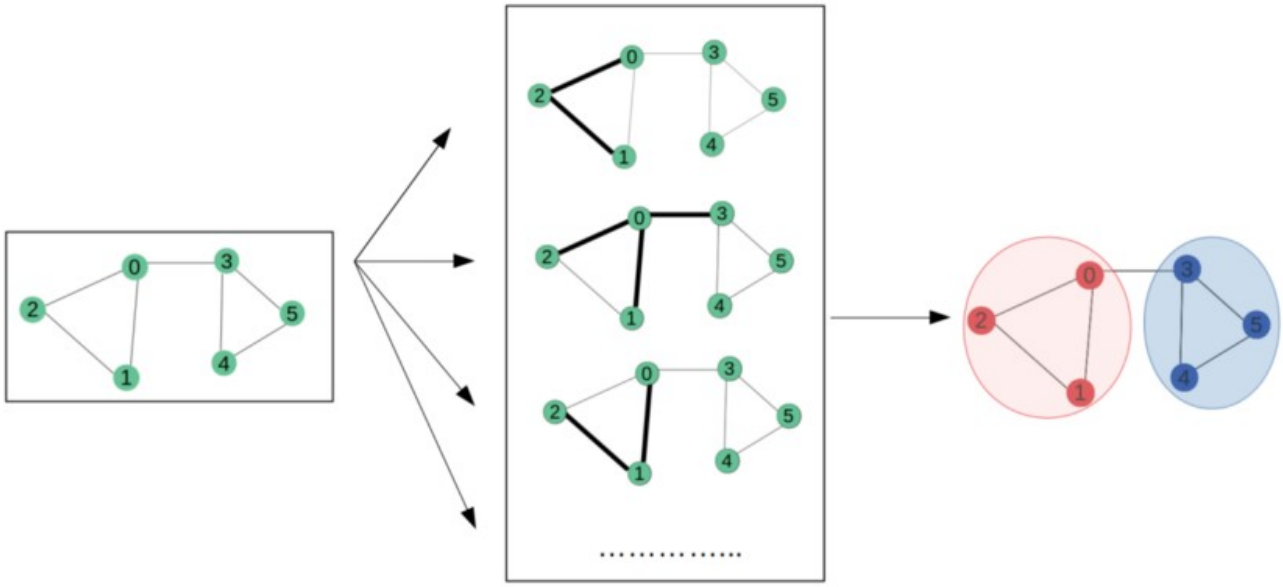


Illustration of Graph Convolutional Networks (image by author)

Neural Networks have gained massive success in the last decade. However, early variants of Neural Networks could only be implemented using regular or Euclidean data, while a lot of data in the real world have underlying graph structures which are non-Euclidean. The non-regularity of data structures have led to recent advancements in Graph Neural

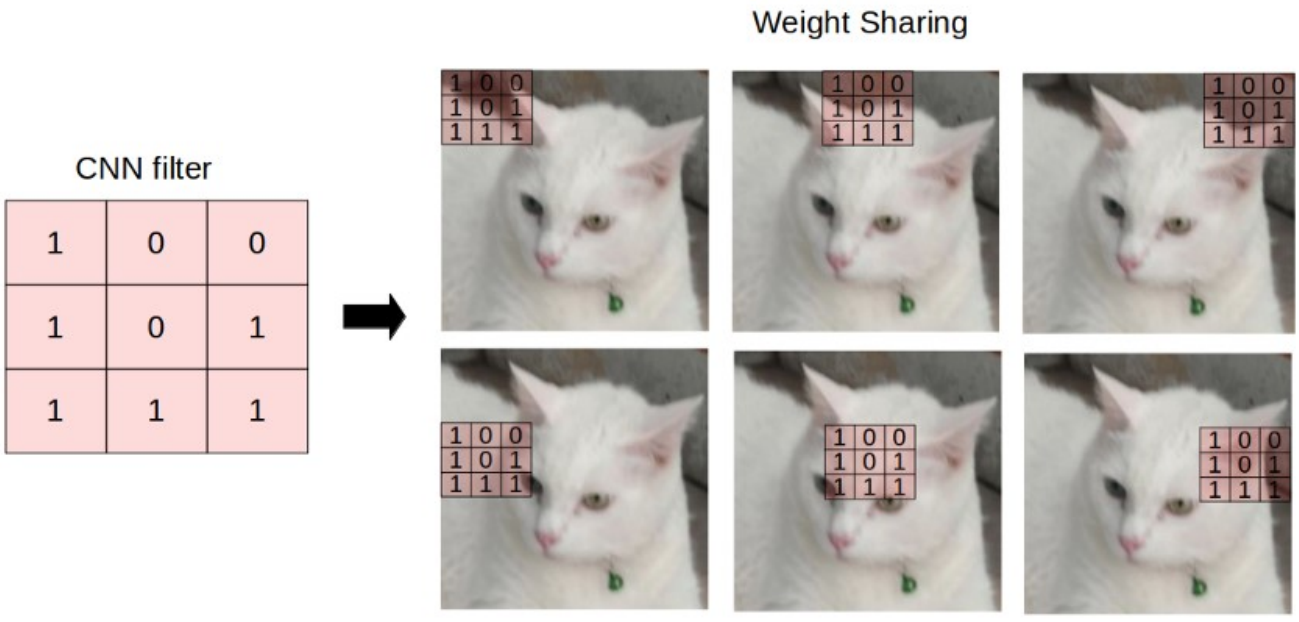
Networks. In the past few years, different variants of Graph Neural Networks are being developed with Graph Convolutional Networks (GCN) being one of them. GCNs are also considered as one of the basic Graph Neural Networks variants.

In this article, we'll dive deeper into Graph Convolutional Networks developed by Thomas Kipf and Max Welling. I will also be giving some very basic examples on building our first graph using NetworkX. By the end of this article, I hope we can gain deeper understanding on the mechanisms inside Graph Convolutional Networks.

If you are not familiar with the basic concepts of Graph Neural Networks, I recommend reading my previous article here.

Convolution in Graph Neural Networks

If you are familiar with convolution layers in Convolutional Neural Networks, 'convolution' in GCNs is basically the same operation. It refers to multiplying the input neurons with a set of weights that are commonly known as *filters* or *kernels*. The filters act as a sliding window across the whole image and enable CNNs to learn features from neighboring cells. Within the same layer, the same filter will be used throughout image, this is referred to as **weight sharing**. For example, using CNN to classify images of cats vs non-cats, the same filter will be used in the same layer to detect the nose and the ears of the cat.



The same weight (or kernel, or filter in CNNs) is applied throughout the image (image by author)

GCNs perform similar operations where the model learns the features by inspecting neighboring nodes. The major difference between CNNs and GNNs is that CNNs are specially built to operate on regular (Euclidean) structured data, while GNNs are the generalized version of CNNs where the numbers of nodes connections vary and the nodes are unordered (irregular on non-Euclidean structured data).

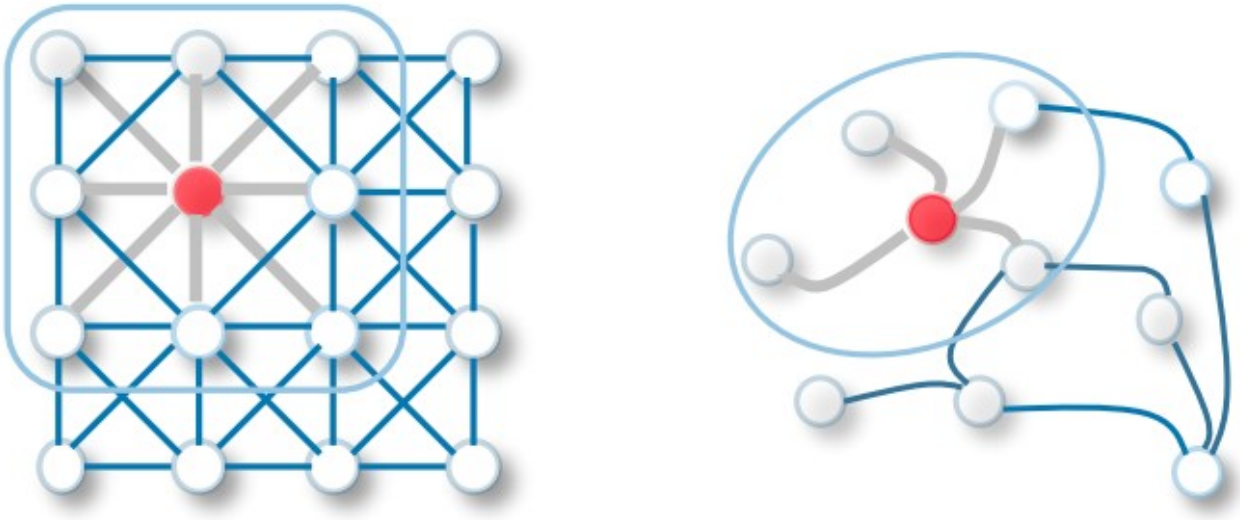


Illustration of 2D Convolutional Neural Networks (left) and Graph Convolutional Networks (right), via source

GCNs themselves can be categorized into 2 major algorithms, **Spatial Graph Convolutional Networks** and **Spectral Graph Convolutional Networks**. In this article, we will be focusing on Fast Approximation Spectral-based Graph Convolutional Networks.

Before diving into the calculations happening inside GCNs, let's briefly recap the concept of forward propagation in Neural Networks first. You can skip the following section if you're familiar with it.

Neural Networks Forward Propagation Brief Recap

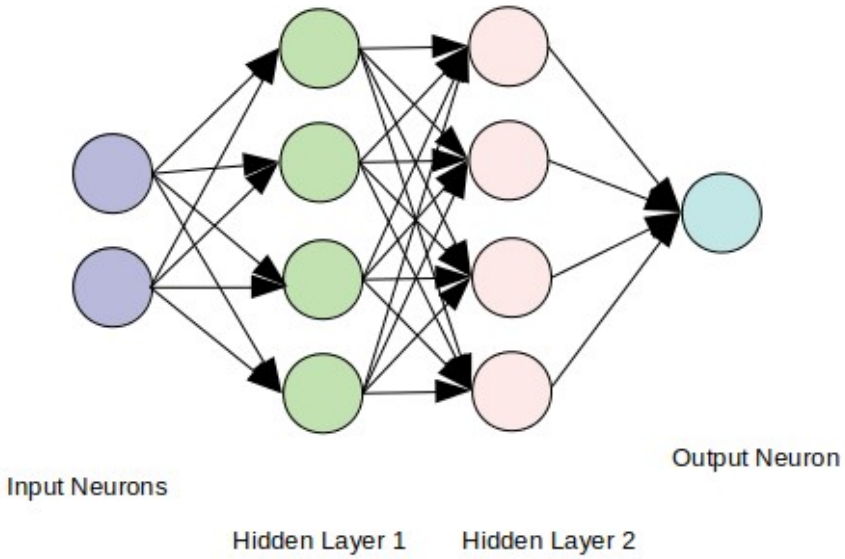


Illustration of Fully-Connected Neural Networks (image by author)

In Neural Networks, in order to propagate the features representation to the next layer (forward pass), we perform the equation below:

$$H^{[i+1]} = \sigma(W^{[i]} H^{[i]} + b^{[i]})$$

- $H^{[i+1]}$: feature representation at layer i+1
- σ: activation function
- $W^{[i]}$: weights at layer i
- $H^{[i]}$: feature representation at layer i
- $b^{[i]}$: bias at layer i

Equation 1 — Forward Pass in Neural Networks

This is basically equivalent to **y = mx+b** in **Linear Regression**, where:

m is equivalent to the **weights**

x is the **input features**

b is the **bias**

What distinguishes the forward pass equation above from Linear Regression is that Neural Networks apply **non-linear activation functions** in order to represent the non-

linear features in latent dimension.

Looking back at the equation above, for the first hidden layer (i = 0), we can simply re-write the equation to be as follows:

$$H^{[1]} = \sigma(W^{T}{}^{[0]} X + b^{[0]})$$

Equation 2 — Forward Pass in Neural Networks at the first layer

where **features representation at layer 0** is basically the **input features (X)**.

How does this equation differ in Graph Convolutional Networks?

Fast Approximate Spectral Graph Convolutional Networks

The original idea behind Spectral GCN was inspired by signal/wave propagation. We can think of information propagation in Spectral GCN as signal propagation along the nodes. Spectral GCNs make use of the Eigen-decomposition of graph Laplacian matrix to implement this method of information propagation. To put it simply, the Eigen-decomposition helps us understand the graph structure, hence, classifying the nodes of the graphs. This is somewhat similar to the basic concept of Principal Component Analysis (PCA) and Linear Discriminant Analysis (LDA) where we use Eigen-decomposition to reduce dimensionality and perform clustering. If you have never heard of Eigen-decomposition and Laplacian matrix, *don't worry!* In this Fast Approximation method, we are not going to use them explicitly.

In this approach, we will take into account the **Adjacency Matrix (A)** in the forward propagation equation in addition to the node features (or so-called input features). **A** is a matrix that represents the edges or connection between the nodes in the forward propagation equation. The insertion of **A** in the forward pass equation enables the model to learn the feature representations based on nodes connectivity. For the sake of simplicity, the bias **b** is omitted. The resulting GCN can be seen as the first-order approximation of Spectral Graph Convolution in the form of a message passing network where the information is propagated along the neighboring nodes within the graph.

By adding the adjacency matrix as an additional element, the forward pass equation will then be:

$$H^{[i+1]} = \sigma(W^{[i]} H^{[i]} A^{*})$$

Equation 3— Forward Pass in Graph Convolutional Networks

*Wait.. You said A, what is **A***?*

A* is the normalized version of **A**. To get better understanding on why we need to normalize **A** and what happens during forward pass in GCNs, let's do an experiment.

Building Graph Convolutional Networks

Initializing the Graph G

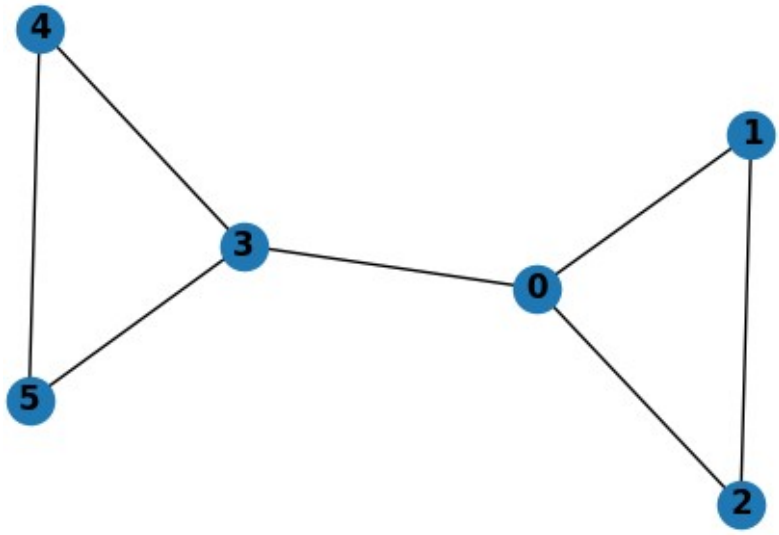
Let's start by building a simple undirected graph (**G**) using NetworkX. The graph **G** will consist of 6 nodes and the feature of each node will correspond to that particular node number. For example, node 1 will have a node feature of 1, node 2 will have a node feature of 2, and so on. To simplify, we are not going to assign edge features in this experiment.

```python
import networkx as nx
import numpy as np
import matplotlib.pyplot as plt
from scipy.linalg import fractional_matrix_power

import warnings
warnings.filterwarnings("ignore", category=UserWarning)


#Initialize the graph
G = nx.Graph(name='G')

#Create nodes
#In this example, the graph will consist of 6 nodes.
#Each node is assigned node feature which corresponds to the node name
for i in range(6):
    G.add_node(i, name=i)


#Define the edges and the edges to the graph
edges = [(0,1),(0,2),(1,2),(0,3),(3,4),(3,5),(4,5)]
G.add_edges_from(edges)

#See graph info
print('Graph Info:\n', nx.info(G))

#Inspect the node features
print('\nGraph Nodes: ', G.nodes.data())

#Plot the graph
nx.draw(G, with_labels=True, font_weight='bold')
plt.show()
```

create_graph.py hosted with ❤ by **GitHub** **view raw**

Output:

```
Graph Info:
 Name: G
Type: Graph
Number of nodes: 6
Number of edges: 7
Average degree:   2.3333

Graph Nodes:  [(0, {'name': 0}), (1, {'name': 1}), (2, {'name': 2}), (3, {'name': 3}), (4, {'name': 4}), (5, {'nam
e': 5})]
```



Graph G visualization

Since we only have 1 graph, this data configuration is an example of a **Single Mode** representation. We will build a GCN that will learn the nodes features representation.

Inserting Adjacency Matrix (A) to Forward Pass Equation

The next step is to obtain the Adjacency Matrix **(A)** and Node Features Matrix **(X)** from graph **G**.

```
#Get the Adjacency Matrix (A) and Node Features Matrix (X) as numpy array
A = np.array(nx.attr_matrix(G, node_attr='name')[0])
X = np.array(nx.attr_matrix(G, node_attr='name')[1])
X = np.expand_dims(X,axis=1)

print('Shape of A: ', A.shape)
print('\nShape of X: ', X.shape)
print('\nAdjacency Matrix (A):\n', A)
print('\nNode Features Matrix (X):\n', X)
```

adj_matrix.py hosted with ❤ by GitHub view raw

Output:

```
Shape of A:  (6, 6)

Shape of X:  (6, 1)

Adjacency Matrix (A):
 [[0. 1. 1. 1. 0. 0.]
 [1. 0. 1. 0. 0. 0.]
 [1. 1. 0. 0. 0. 0.]
 [1. 0. 0. 0. 1. 1.]
 [0. 0. 0. 1. 0. 1.]
 [0. 0. 0. 1. 1. 0.]]

Node Features Matrix (X):
 [[0]
 [1]
 [2]
 [3]
 [4]
 [5]]
```

Now, let's investigate how by inserting **A** into the forward pass equation adds to richer feature representation of the model. We are going to perform dot product of **A** and **X.** Let's call the result of this dot product operation as *AX* in this article.

```
#Dot product Adjacency Matrix (A) and Node Features (X)
AX = np.dot(A,X)
print("Dot product of A and X (AX):\n", AX)
```

dot_prod.py hosted with ❤ by **GitHub** **view raw**

Output:

```
Dot product of A and X (AX):
 [[6.]
 [2.]
 [1.]
 [9.]
 [8.]
 [7.]]
```

From the results, it is apparent that *AX* represents the **sum of neighboring nodes features.** For example, the first row of *AX* corresponds to the sum of nodes features connected to node 0, which is node 1, 2, and 3. This gives us an idea how the propagation mechanism is happening in GCNs and how the node connectivity impacts the hidden features representation seen by GCNs.

> *The dot product of Adjacency Matrix and Node Features Matrix represents the sum of neighboring node features.*

But, if we think about it more, we will realize that while *AX* sums up the adjacent node

features, **it does not take into account the features of the node itself.**

Oops, problem detected! How to solve it?

Inserting Self-Loops and Normalizing A

To address this problem, we now add self-loops to each node of **A.** Adding self-loops is basically a mechanism to connect a node to itself. That being said, all the diagonal elements of Adjacency Matrix **A** will now become 1 because each node is connected to itself. Let's call **A** with self-loops added as **A_hat** and recalculate *AX*, which is now the dot product of **A_hat** and **X**:

```
#Add Self Loops
G_self_loops = G.copy()

self_loops = []
for i in range(G.number_of_nodes()):
    self_loops.append((i,i))

G_self_loops.add_edges_from(self_loops)

#Check the edges of G_self_loops after adding the self loops
print('Edges of G with self-loops:\n', G_self_loops.edges)

#Get the Adjacency Matrix (A) and Node Features Matrix (X) of added self-lopps graph
A_hat = np.array(nx.attr_matrix(G_self_loops, node_attr='name')[0])
print('Adjacency Matrix of added self-loops G (A_hat):\n', A_hat)

#Calculate the dot product of A_hat and X (AX)
AX = np.dot(A_hat, X)
print('AX:\n', AX)
```

self_loop.py hosted with ❤ by GitHub view raw

Output:

```
Edges of G with self-loops:
 [(0, 1), (0, 2), (0, 3), (0, 0), (1, 2), (1, 1), (2, 2), (3, 4), (3, 5), (3, 3), (4, 5), (4, 4), (5, 5)]
Adjacency Matrix of added self-loops G (A_hat):
 [[1. 1. 1. 1. 0. 0.]
 [1. 1. 1. 0. 0. 0.]
 [1. 1. 1. 0. 0. 0.]
 [1. 0. 0. 1. 1. 1.]
 [0. 0. 0. 1. 1. 1.]
 [0. 0. 0. 1. 1. 1.]]
AX:
 [[ 6.]
 [ 3.]
 [ 3.]
 [12.]
 [12.]
 [12.]]
```

Great! One problem solved!

Now, you might recognize another problem. The elements of *AX* are **not normalized**. Similar to data pre-processing for any Neural Networks operation, we need to normalize the features to prevent numerical instabilities and vanishing/exploding gradients in order for the model to converge. In GCNs, we normalize our data by **calculating the Degree Matrix (D) and performing dot product operation of the inverse of D with** *AX*

$$\text{normalized features} = D^{-1}AX$$

which we will call *DAX* in this article. In graph terminology, the term “degree” refers to the number of edges a node is connected to.

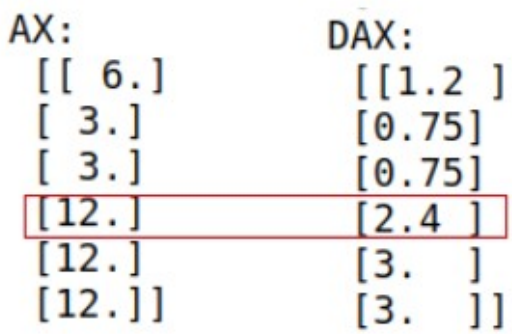
```python
#Get the Degree Matrix of the added self-loops graph
Deg_Mat = G_self_loops.degree()
print('Degree Matrix of added self-loops G (D): ', Deg_Mat)

#Convert the Degree Matrix to a N x N matrix where N is the number of nodes
D = np.diag([deg for (n,deg) in list(Deg_Mat)])
print('Degree Matrix of added self-loops G as numpy array (D):\n', D)

#Find the inverse of Degree Matrix (D)
D_inv = np.linalg.inv(D)
print('Inverse of D:\n', D_inv)

#Dot product of D and AX for normalization
DAX = np.dot(D_inv,AX)
print('DAX:\n', DAX)
```

degree_mat.py hosted with ❤ by **GitHub** **view raw**

Output:

```
Degree Matrix of added self-loops G (D):  [(0, 5), (1, 4), (2, 4), (3, 5), (4, 4), (5, 4)]
Degree Matrix of added self-loops G as numpy array (D):
 [[5 0 0 0 0 0]
 [0 4 0 0 0 0]
 [0 0 4 0 0 0]
 [0 0 0 5 0 0]
 [0 0 0 0 4 0]
 [0 0 0 0 0 4]]
Inverse of D:
 [[0.2  0.   0.   0.   0.   0.  ]
 [0.   0.25 0.   0.   0.   0.  ]
 [0.   0.   0.25 0.   0.   0.  ]
 [0.   0.   0.   0.2  0.   0.  ]
 [0.   0.   0.   0.   0.25 0.  ]
 [0.   0.   0.   0.   0.   0.25]]
DAX:
 [[1.2 ]
 [0.75]
 [0.75]
 [2.4 ]
 [3.  ]
 [3.  ]]
```

If we compare *DAX* with *AX*, we will notice that:



We can see the impact normalization has on DAX, where the element that corresponds to node 3 has lower values compared to node 4 and 5. But why would node 3 have different values after normalization if it has the same initial value as node 4 and 5?

Let's take a look back at our graph. Node 3 has **3 incident edges**, while nodes 4 and 5 only have **2 incident edges**. The fact that **node 3 has a higher degree** than node 4 and 5 leads to a **lower weighting of node 3's features in *DAX***. In other words, the lower the degree of a node, the stronger that a node belongs to a certain group or cluster.

In the paper, Kipf and Welling states that doing symmetric normalization will make dynamics more interesting, hence, the normalization equation is modified from:

$$\text{normalizing term} = D^{-1} A$$

to

$$\text{normalizing term} = D^{-1/2} A D^{-1/2}$$

Let's calculate the normalized values using the new symmetric normalization equation:

```
#Symmetrically-normalization
D_half_norm = fractional_matrix_power(D, -0.5)
DADX = D_half_norm.dot(A_hat).dot(D_half_norm).dot(X)
print('DADX:\n', DADX)
```

sym_norm.py hosted with ❤ by GitHub view raw

Output:

```
DADX:
 [[1.27082039]
 [0.75      ]
 [0.75      ]
 [2.61246118]
 [2.92082039]
 [2.92082039]]
```

Looking back at Equation 3 in the previous section, we will realize that we now have the answers to what is **A***! In the paper, **A*** is referred to as *renormalization trick*.

Having finished with features handling, it's time to finalize our GCN.

Adding Weights and Activation Function

We are going to build a 2-layer GCN using ReLu as the activation function. To initialize the weights, we will use random seeds so we can replicate the results. Just keep in mind that the weight initialization cannot be 0. In this experiment, we are going to set 4 neurons for the hidden layer. As we will be plotting the feature representations in 2 dimensions, there will be 2 output neurons.

Just to make it simpler, we will re-write the *renormalization trick* equation using numpy, just to make it simpler.

```python
#Initialize the weights
np.random.seed(77777)
n_h = 4 #number of neurons in the hidden layer
n_y = 2 #number of neurons in the output layer
W0 = np.random.randn(X.shape[1],n_h) * 0.01
W1 = np.random.randn(n_h,n_y) * 0.01

#Implement ReLu as activation function
def relu(x):
    return np.maximum(0,x)

#Build GCN layer
#In this function, we implement numpy to simplify
def gcn(A,H,W):
    I = np.identity(A.shape[0]) #create Identity Matrix of A
    A_hat = A + I #add self-loop to A
    D = np.diag(np.sum(A_hat, axis=0)) #create Degree Matrix of A
    D_half_norm = fractional_matrix_power(D, -0.5) #calculate D to the power of -0.5
    eq = D_half_norm.dot(A_hat).dot(D_half_norm).dot(H).dot(W)
    return relu(eq)


#Do forward propagation
H1 = gcn(A,X,W0)
H2 = gcn(A,H1,W1)
print('Features Representation from GCN output:\n', H2)
```

build_gcn.py hosted with ❤ by GitHub view raw

Any comment, feedback, or want to discuss? Just drop me a message. You can reach me on LinkedIn.

Output:

You can get the full code on GitHub.

```
Features Representation from GCN output:
 [[0.00027758 0.        ]
 [0.00017298 0.        ]
 [0.00017298 0.        ]
 [0.00053017 0.        ]
 [0.00054097 0.        ]
 [0.00054097 0.        ]]
```

Done! We have just built our first feed-forward GCN model!

Plotting the Features Representations

The 'magic' of GCN is that it can learn features representation even without training.

Let's visualize the features representations after passing through 2-layer GCN.

Networks (2019). arXiv preprint arXiv:1609.02907. ICLR 2017)

[2] T. Kipf, https://tkipf.github.io/graph-convolutional-networks/

[3] Z. Wu, et. al., A Comprehensive Survey on Graph Neural Networks (2019).

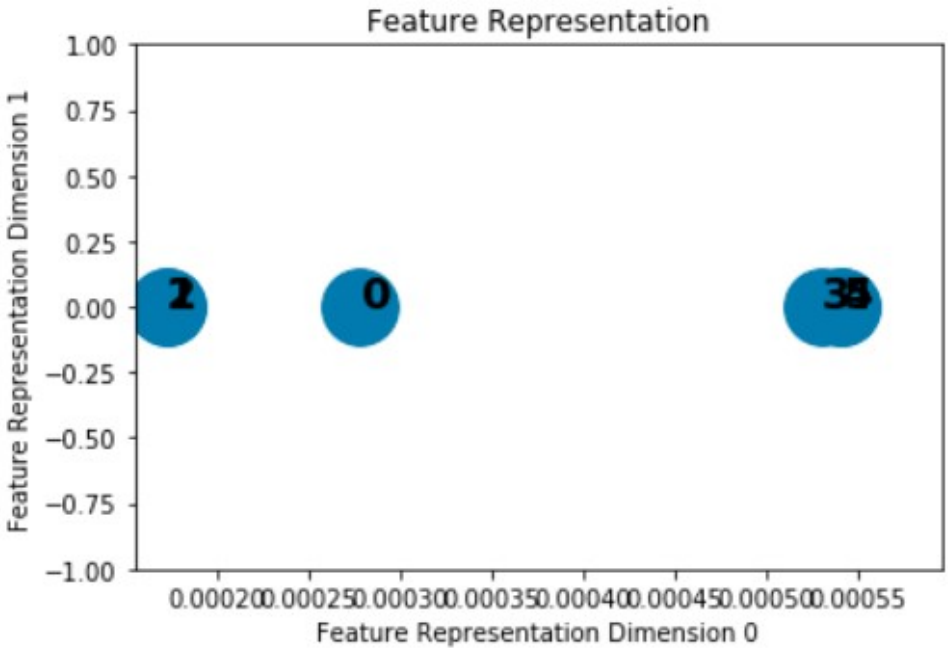
[4] T. S. Jepsen, https://towardsdatascience.com/how-to-do-deep-learning-on-graphs-

with-graph-convolutional-networks-7d2250723780

```python
def plot_features(H2):
    #Plot the features representation
    x = H2[:,0]
    y = H2[:,1]

    size = 1000

    plt.scatter(x,y,size)
    plt.xlim([np.min(x)*0.9, np.max(x)*1.1])
    plt.ylim([-1, 1])
    plt.xlabel('Feature Representation Dimension 0')
    plt.ylabel('Feature Representation Dimension 1')
    plt.title('Feature Representation')

    for i,row in enumerate(H2):
        str = "{}".format(i)
        plt.annotate(str, (row[0],row[1]),fontsize=18, fontweight='bold')

    plt.show()


plot_features(H2)
```

plot_features.py hosted with ❤ by GitHub view raw

Output:



Features Representation from Feed-Forward GCN

From the plot above, it can be clearly seen that there are 2 major groups, where the left group consists of nodes 0, 1, 2, and the right group consists of nodes 3, 4, 5. We can infer that the **GC can already learn the feature representations even without training or backpropagation**

Key Takeaways

- The term 'convolution' in Graph Convolutional Networks is similar to Convolutional Neur Networks in terms of *weight sharing*. The main difference lies in the data structure, where GCNs are the generalized version of CNN that can work on data with underlying non-regu structures.
- The insertion of Adjacency Matrix (**A**) in the forward pass equation of GCNs enable the model to learn the features of neighboring nodes. This mechanism can be seen as a messa passing operation along the nodes within the graph.
- *Renormalization trick* is used to normalize the features in Fast Approximate Spectral-base Graph Convolutional Networks by Thomas Kipf and Max Welling (2017).
- GCNs can learn features representation even before training.