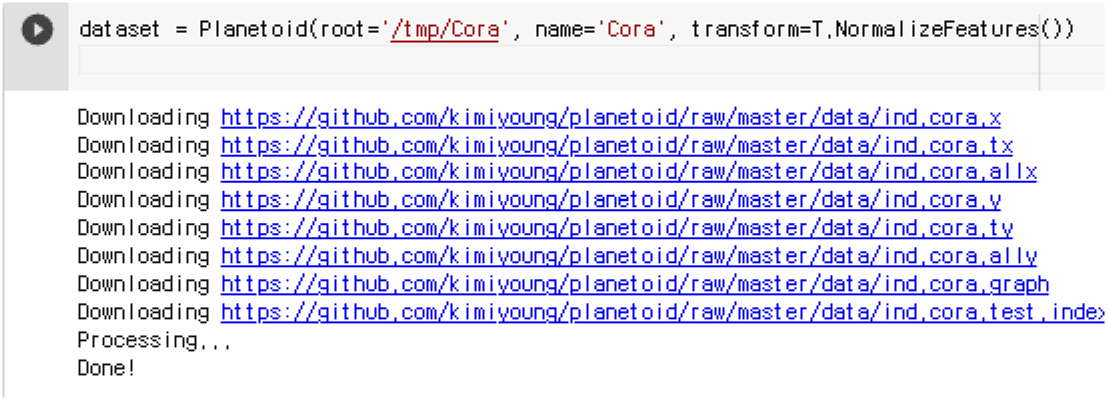
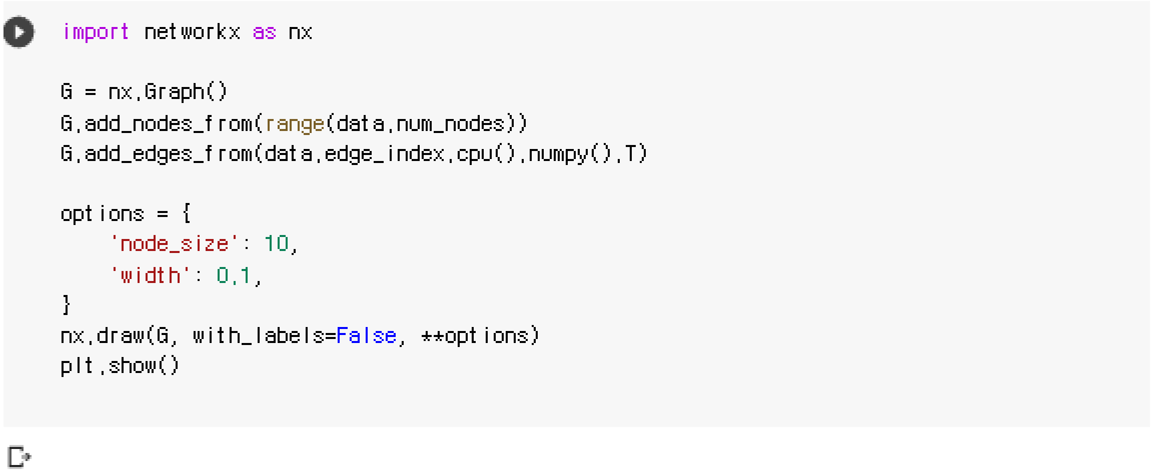
1) Dataset

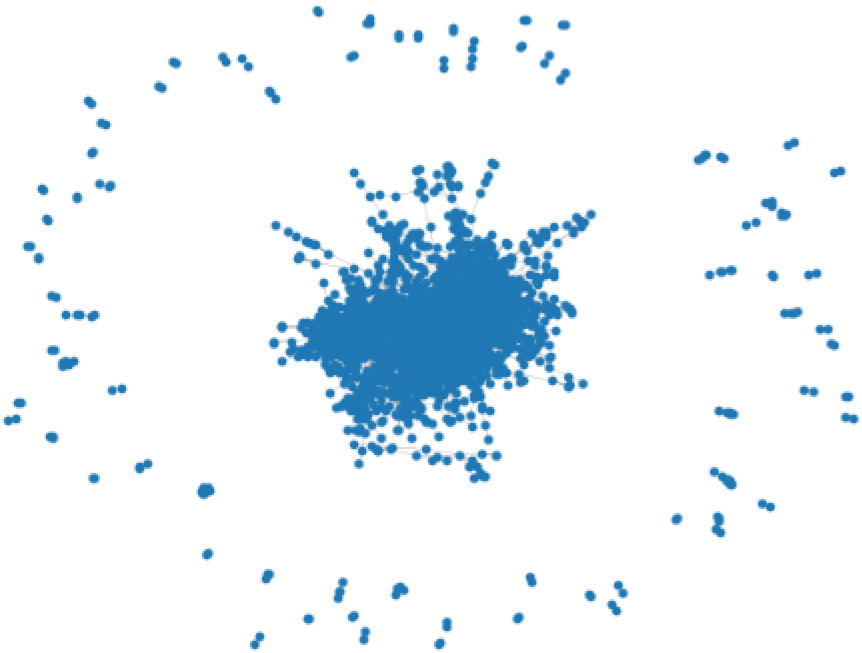


```
dataset = Planetoid(root='/tmp/Cora', name='Cora', transform=T.NormalizeFeatures())
```

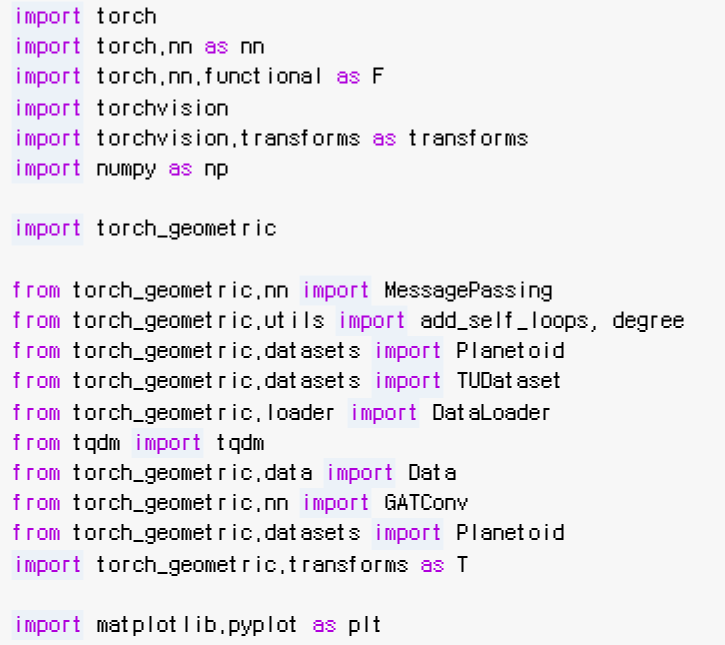
```
Downloading https://github.com/kimiyoung/planetoid/raw/master/data/ind.cora.x
Downloading https://github.com/kimiyoung/planetoid/raw/master/data/ind.cora.tx
Downloading https://github.com/kimiyoung/planetoid/raw/master/data/ind.cora.allx
Downloading https://github.com/kimiyoung/planetoid/raw/master/data/ind.cora.y
Downloading https://github.com/kimiyoung/planetoid/raw/master/data/ind.cora.ty
Downloading https://github.com/kimiyoung/planetoid/raw/master/data/ind.cora.ally
Downloading https://github.com/kimiyoung/planetoid/raw/master/data/ind.cora.graph
Downloading https://github.com/kimiyoung/planetoid/raw/master/data/ind.cora.test.inde
Processing...
Done!
```



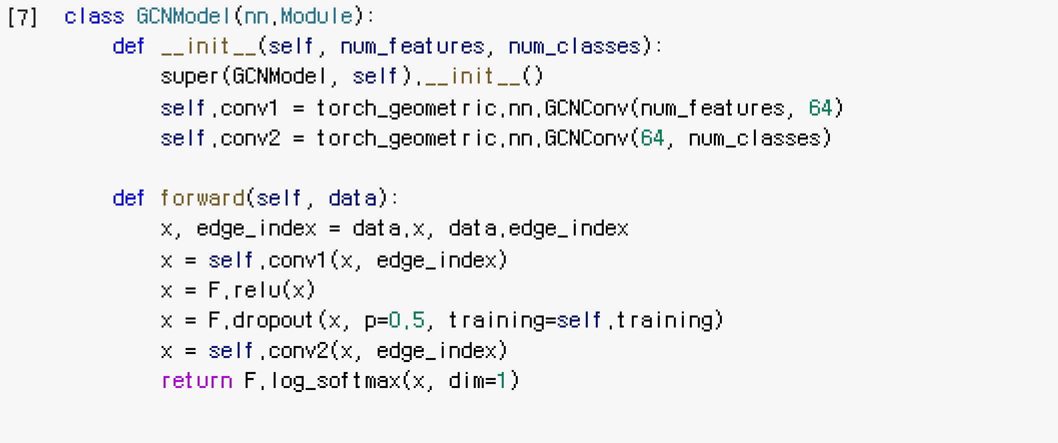
```
import networkx as nx

G = nx.Graph()
G.add_nodes_from(range(data.num_nodes))
G.add_edges_from(data.edge_index.cpu().numpy().T)

options = {
    'node_size': 10,
    'width': 0.1,
}
nx.draw(G, with_labels=False, **options)
plt.show()
```



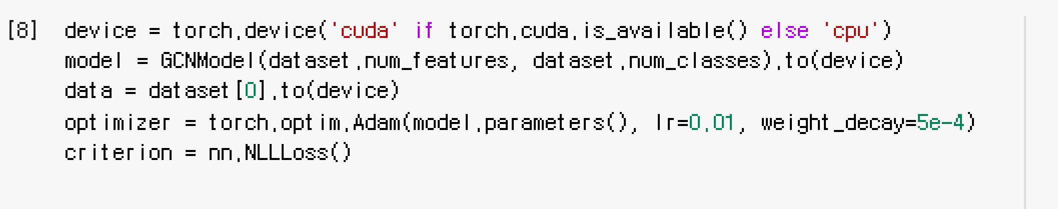
2) Setup & define a GNN model (loss function, activation function; optimizer)



```
import torch
import torch.nn as nn
import torch.nn.functional as F
import torchvision
import torchvision.transforms as transforms
import numpy as np

import torch_geometric

from torch_geometric.nn import MessagePassing
from torch_geometric.utils import add_self_loops, degree
from torch_geometric.datasets import Planetoid
from torch_geometric.datasets import TUDataset
from torch_geometric.loader import DataLoader
from tqdm import tqdm
from torch_geometric.data import Data
from torch_geometric.nn import GATConv
from torch_geometric.datasets import Planetoid
import torch_geometric.transforms as T

import matplotlib.pyplot as plt
```

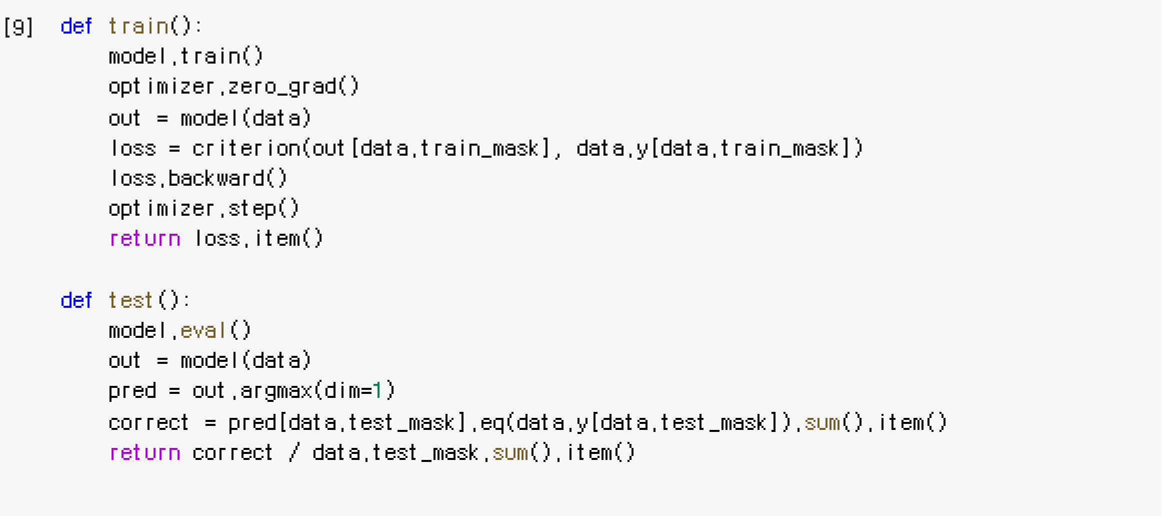


```
[7]  class GCNModel(nn.Module):
         def __init__(self, num_features, num_classes):
             super(GCNModel, self).__init__()
             self.conv1 = torch_geometric.nn.GCNConv(num_features, 64)
             self.conv2 = torch_geometric.nn.GCNConv(64, num_classes)

         def forward(self, data):
             x, edge_index = data.x, data.edge_index
             x = self.conv1(x, edge_index)
             x = F.relu(x)
             x = F.dropout(x, p=0.5, training=self.training)
             x = self.conv2(x, edge_index)
             return F.log_softmax(x, dim=1)
```

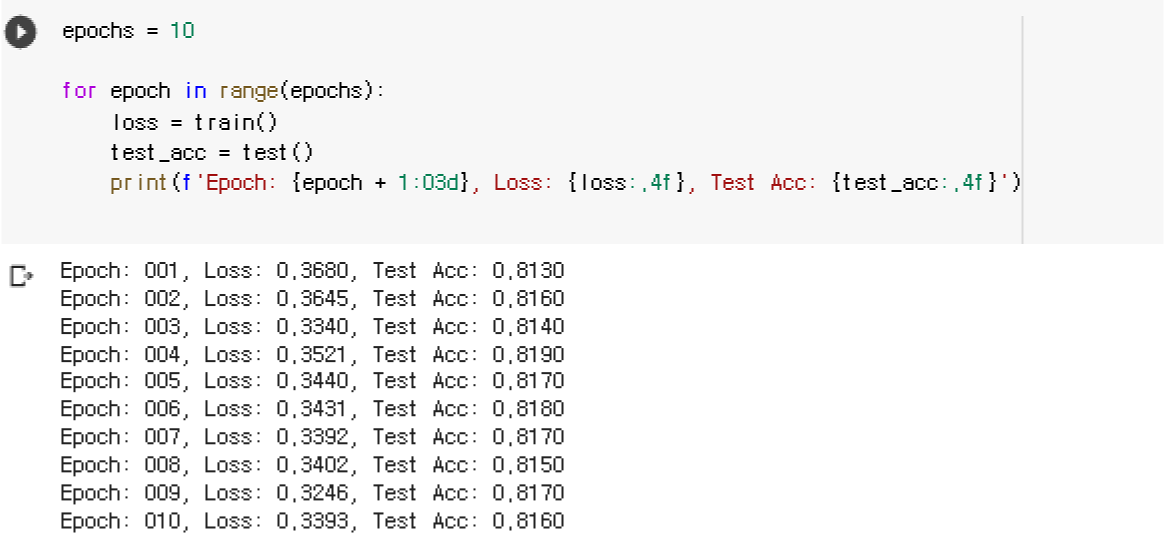


```
[8]  device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
     model = GCNModel(dataset.num_features, dataset.num_classes).to(device)
     data = dataset[0].to(device)
     optimizer = torch.optim.Adam(model.parameters(), lr=0.01, weight_decay=5e-4)
     criterion = nn.NLLLoss()
```

3) Model training & testing



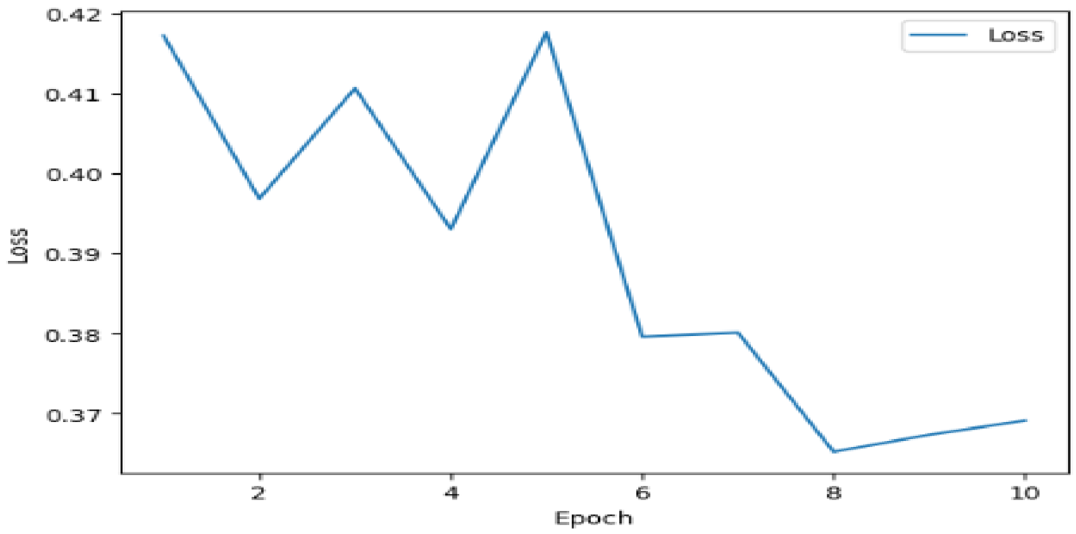
```
[9] def train():
        model.train()
        optimizer.zero_grad()
        out = model(data)
        loss = criterion(out[data.train_mask], data.y[data.train_mask])
        loss.backward()
        optimizer.step()
        return loss.item()

    def test():
        model.eval()
        out = model(data)
        pred = out.argmax(dim=1)
        correct = pred[data.test_mask].eq(data.y[data.test_mask]).sum().item()
        return correct / data.test_mask.sum().item()
```

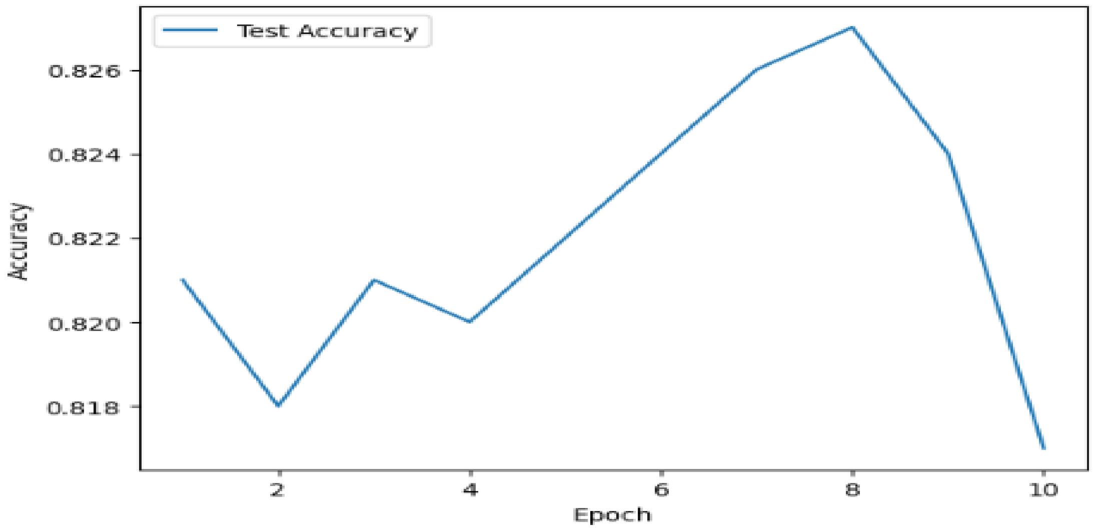


```
epochs = 10

for epoch in range(epochs):
    loss = train()
    test_acc = test()
    print(f'Epoch: {epoch + 1:03d}, Loss: {loss:.4f}, Test Acc: {test_acc:.4f}')
```

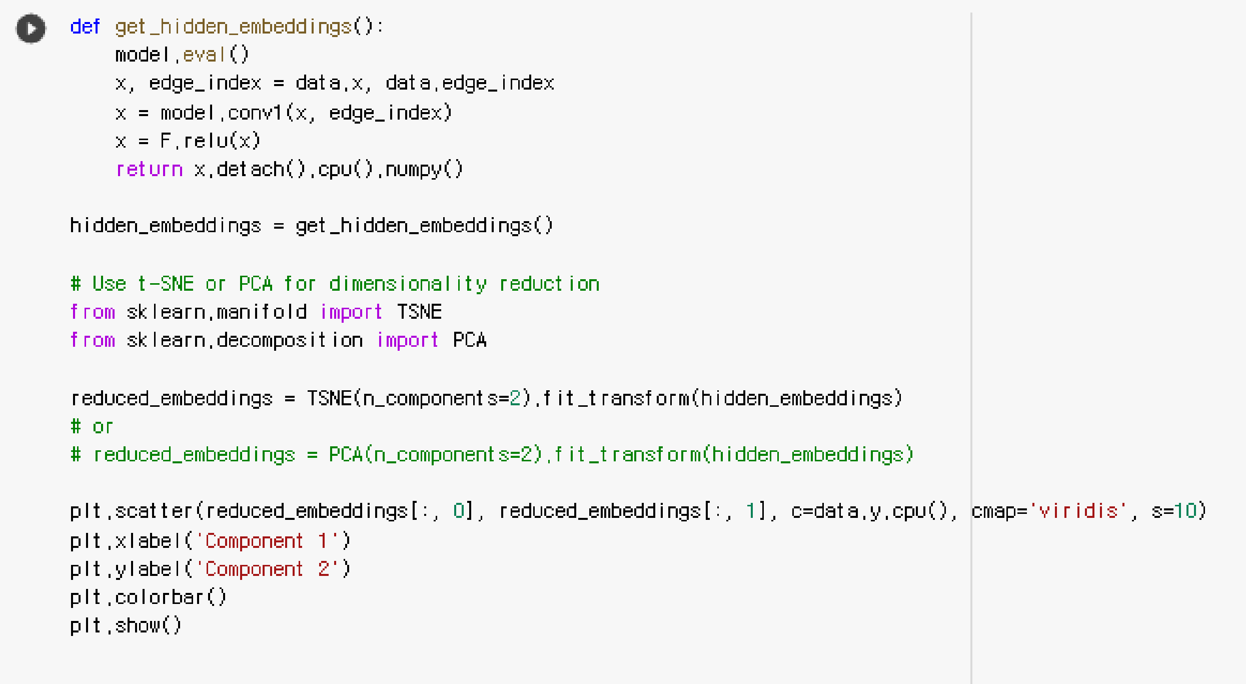
```
Epoch: 001, Loss: 0.3680, Test Acc: 0.8130
Epoch: 002, Loss: 0.3645, Test Acc: 0.8160
Epoch: 003, Loss: 0.3340, Test Acc: 0.8140
Epoch: 004, Loss: 0.3521, Test Acc: 0.8190
Epoch: 005, Loss: 0.3440, Test Acc: 0.8170
Epoch: 006, Loss: 0.3431, Test Acc: 0.8180
Epoch: 007, Loss: 0.3392, Test Acc: 0.8170
Epoch: 008, Loss: 0.3402, Test Acc: 0.8150
Epoch: 009, Loss: 0.3246, Test Acc: 0.8170
Epoch: 010, Loss: 0.3393, Test Acc: 0.8160
```

```
2]  loss_history = []
    test_acc_history = []

    epochs = 10

    for epoch in range(epochs):
        loss = train()
        test_acc = test()
        loss_history.append(loss)
        test_acc_history.append(test_acc)

    plt.figure()
    plt.plot(range(1, epochs + 1), loss_history, label='Loss')
    plt.xlabel('Epoch')
    plt.ylabel('Loss')
    plt.legend()
    plt.show()

    plt.figure()
    plt.plot(range(1, epochs + 1), test_acc_history, label='Test Accuracy')
    plt.xlabel('Epoch')
    plt.ylabel('Accuracy')
    plt.legend()
    plt.show()
```

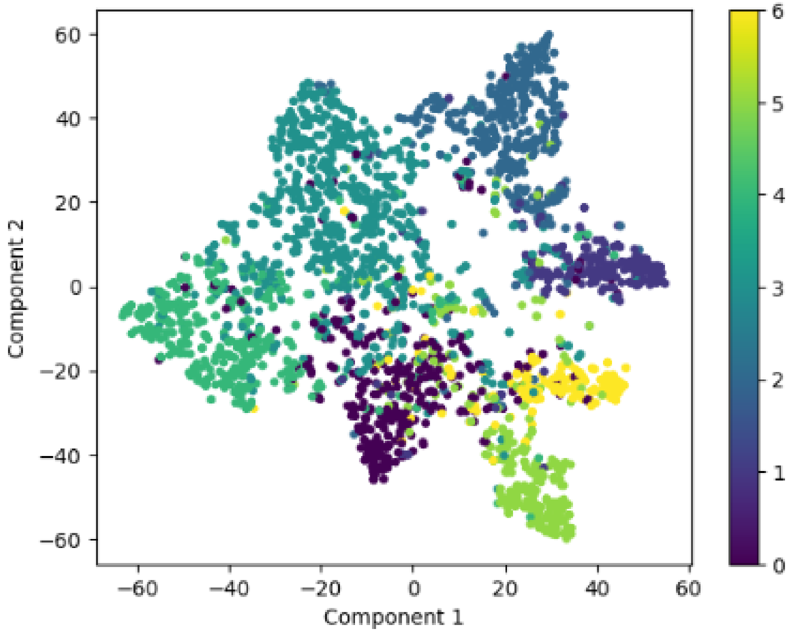




4) PCA of GCN



```
def get_hidden_embeddings():
    model.eval()
    x, edge_index = data.x, data.edge_index
    x = model.conv1(x, edge_index)
    x = F.relu(x)
    return x.detach().cpu().numpy()

hidden_embeddings = get_hidden_embeddings()

# Use t-SNE or PCA for dimensionality reduction
from sklearn.manifold import TSNE
from sklearn.decomposition import PCA

reduced_embeddings = TSNE(n_components=2).fit_transform(hidden_embeddings)
# or
# reduced_embeddings = PCA(n_components=2).fit_transform(hidden_embeddings)

plt.scatter(reduced_embeddings[:, 0], reduced_embeddings[:, 1], c=data.y.cpu(), cmap='viridis', s=10)
plt.xlabel('Component 1')
plt.ylabel('Component 2')
plt.colorbar()
plt.show()
```


Component 2
Component 1