Node Classification in Citation Networks using Graph Convolutional Networks

As part of the **BTech Summer Internship Program**

Submitted by:
Harsh Lad
Student ID : 202201493
B tech- Information and Communication Technology

Under the guidance of:
Prof. Manoj Raut

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Abstract

This research project, conducted as part of the **BTech Summer Internship Program**, investigates the use of Graph Convolutional Networks (GCNs) for node classification in citation networks. Citation networks represent academic papers as nodes and citations as edges, forming a structured graph. The goal is to predict the topic or category of a research paper based on its content features and citation relationships.

We utilize two widely-used benchmark datasets — **Cora** and **Citeseer** — both of which contain labeled papers with feature vectors and citation links. A two-layer GCN is implemented using PyTorch Geometric to learn node embeddings that combine both textual features and graph structure. The model is trained in a semi-supervised setting, where only a portion of the nodes have known labels.

Performance is evaluated using classification metrics such as accuracy, precision, recall, and F1-score. Additionally, we apply t-SNE for visualizing the learned embeddings, showing how the GCN clusters similar papers in the feature space. Our results demonstrate that GCNs significantly outperform traditional models by effectively leveraging both node features and neighborhood information in the graph.

This project showcases the strength of graph-based learning in understanding structured data and offers a foundation for future work in citation analysis, research paper recommendation, and graph-based machine learning.

1 Introduction :

In recent years, graph-structured data has become increasingly important across various domains such as social networks, biological networks, and citation networks. Traditional machine learning models often struggle to work with graph data, as they are primarily designed for tabular or sequential formats. To address this challenge, Graph Neural Networks (GNNs) have emerged as powerful models capable of learning from the structure and features of graphs.

This research project focuses on the problem of **node classification** in citation networks using a type of GNN known as the **Graph Convolutional Network (GCN)**. In a citation network, each node represents a research paper, and an edge between two nodes indicates a citation relationship. The goal is to predict the topic or subject area of a research paper based on its content features and the structure of citations in the network.

We use two widely studied benchmark datasets — **Cora** and **Citeseer** — where each paper is represented by a sparse feature vector (based on the words it contains), and is assigned a label indicating its research area. These datasets also provide citation links, forming a graph suitable for GNN-based learning.

In this project, we implement a two-layer GCN to perform semi-supervised node classification. The GCN aggregates information from a node's neighbors and updates its representation based on both the local graph structure and node features. We train the model using a small subset

of labeled nodes and evaluate its performance using classification accuracy, confusion matrix, and t-SNE visualizations of learned node embeddings.

Through this work, we demonstrate how GCNs can effectively leverage graph topology to enhance classification performance, outperforming simple models that do not consider the citation structure.

2 Review of Existing Methods :

Graph Neural Networks (GNNs) have become a powerful framework for learning from graph-structured data. Among the earliest and most influential models is the **Graph Convolutional Network (GCN)** proposed by Kipf and Welling [2], which applies spectral convolution operations for semi-supervised node classification.

Since then, many variants such as Graph Attention Networks (GAT) [4] and GraphSAGE [1] have extended the GCN approach by incorporating attention and inductive learning, respectively.

The Cora and Citeseer datasets have been widely used to benchmark GNN models. Prior works demonstrate that incorporating graph structure improves classification accuracy compared to models that rely only on node features.

Our project builds on these foundations by implementing a two-layer GCN using PyTorch Geometric and evaluating its performance on node classification in citation networks.

3 Datasets :

This project uses two benchmark citation network datasets: **Cora** and **Citeseer**, both available via the PyTorch Geometric `Planetoid` loader. Each node in these datasets represents a research paper described by a sparse bag-of-words feature vector, and each edge represents a citation between papers. The goal is to classify each paper into one of several predefined research areas.

→ **Cora Dataset**

- **Number of nodes:** 2708
- **Number of edges:** 5278 (undirected)
- **Features per node:** 1433
- **Number of classes:** 7
- **Isolated nodes:** No
- **Self-loops:** No

- **Graph density:** 0.00144
- **Connected components:** 78
- **Largest component:** 2485 nodes (91.77% of the graph)
- **Average node degree:** 3.90

→ **Citeseer Dataset**

- **Number of nodes:** 3279
- **Number of edges:** 4552 (undirected)
- **Features per node:** 3703
- **Number of classes:** 6
- **Isolated nodes:** Yes
- **Self-loops:** No
- **Graph density:** 0.00085
- **Connected components:** 390
- **Largest component:** 2120 nodes (64.65% of the graph)
- **Average node degree:** 2.78

→ **Train, Validation, and Test Splits**

Both datasets follow a standard semi-supervised split:

- **Training nodes:** 140 (Cora), 120 (Citeseer)
- **Validation nodes:** 500
- **Test nodes:** 1000

→ **Node Degree Distributions**

To understand the graph structure, we plotted the **node degree distribution** (i.e., number of nodes having a given degree). These plots confirm that both datasets are sparse and follow a long-tail distribution — a few nodes have high degree (frequent citations), while most nodes are weakly connected.

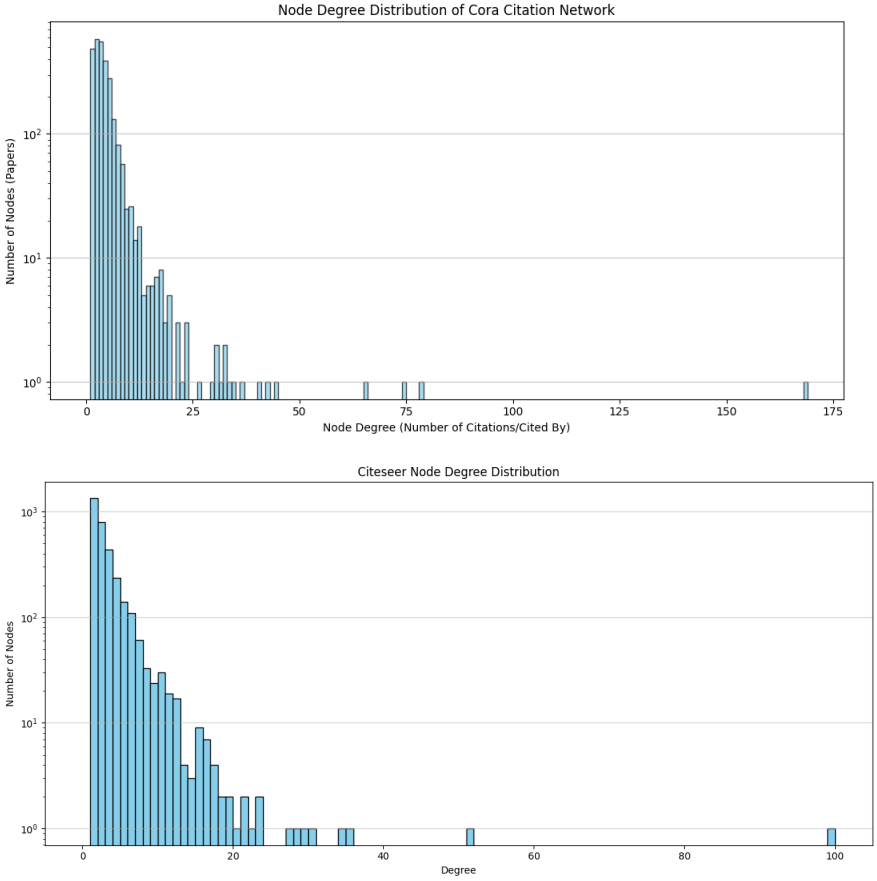

Figure 1: Node Degree Distribution: Cora (1st) and Citeseer (2nd). Y-axis is in log scale.

These graphs validate the real-world nature of citation networks: they are sparse, partially disconnected (especially Citeseer), and follow power-law-like behavior, which makes them well-suited for graph neural network models.

4 Architecture Overview :

→ The architecture of our system is designed to perform node classification over citation networks using a Graph Convolutional Network (GCN). The process starts with loading a citation graph, followed by passing the node features and graph structure through stacked GCN layers. The model aggregates information from each node's neighborhood and finally outputs class probabilities for each node.

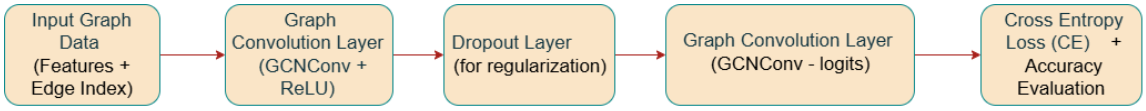

Figure 2: End-to-end pipeline for node classification using GCN. The architecture includes input graph data (features and edges), two GCN layers with ReLU and Dropout, and classification output using softmax over node embeddings.

The figure above illustrates the complete architecture pipeline implemented in the project.

5 Methodology :

Our approach consists of applying a Graph Convolutional Network (GCN) to perform node classification on citation network datasets. The methodology can be broken down into four primary stages: dataset preparation, GCN model design, training and evaluation, and embedding visualization.

5.1 Dataset Preparation

→ We use the publicly available **Cora** and **Citeseer** citation networks provided by the `torch_geometric.datasets.Planetoid` loader. Each dataset consists of:

- A sparse feature matrix $\mathbf{X} \in \mathbb{R}^{N \times F}$, where N is the number of nodes (papers) and F is the number of input features.
- An edge index $\mathbf{E}$ representing citation relationships as a list of directed edges.
- A label vector $\mathbf{Y} \in \{1, 2, ..., C\}^N$ indicating the topic category for each paper, where C is the number of classes.

5.2 GCN Model Design

→ We implement a two-layer Graph Convolutional Network as proposed by Kipf and Welling [2]. The forward pass of the model is defined as:

$$\mathbf{H}^{(1)} = \text{ReLU}\left(\hat{\mathbf{A}}\mathbf{X}\mathbf{W}^{(0)}\right)$$

$$\mathbf{H}^{(2)} = \hat{\mathbf{A}}\mathbf{H}^{(1)}\mathbf{W}^{(1)}$$

where $\hat{\mathbf{A}}$ is the normalized adjacency matrix with self-loops, $\mathbf{W}^{(0)}$ and $\mathbf{W}^{(1)}$ are learnable weight matrices, and ReLU is the activation function. The final layer outputs logits for each class per node.

The model is trained using cross-entropy loss applied only to the nodes in the training set.

→ We implement a two-layer Graph Convolutional Network using PyTorch Geometric to classify nodes in a citation graph. The network takes in node features and performs neighborhood aggregation over the graph structure.

The model is defined as:

```
class GCN(torch.nn.Module):
    def __init__(self, in_channels, hidden_channels, out_channels)
        :
        super().__init__()
        torch.manual_seed(12345)
        self.conv1 = GCNConv(in_channels, hidden_channels)
        self.conv2 = GCNConv(hidden_channels, out_channels)

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

Listing 1: GCN Model Architecture

The model is initialized with input, hidden, and output dimensions based on dataset parameters, and optimized using the Adam optimizer:

```
model = GCN(data.num_node_features, 16, dataset.num_classes)
optimizer = torch.optim.Adam(model.parameters(), lr=0.01)
criterion = torch.nn.CrossEntropyLoss()
```

Listing 2: Model Initialization and Loss

5.3 Training and Evaluation

→ We use the Adam optimizer with a learning rate of 0.01. The model is trained for 400 epochs. Dropout is applied after the first layer to prevent overfitting.

Evaluation is performed using the test set, and metrics such as accuracy, precision, recall, and F1-score are reported using a classification report and confusion matrix.

→ The training process involves forward propagation through the GCN, computation of cross-entropy loss, backpropagation, and parameter updates. Evaluation is done using test accuracy.

Training and testing functions are defined as follows:

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

def test():
    model.eval()
    with torch.no_grad():
        out = model(data.x, data.edge_index)
    pred = out.argmax(dim=1)
    correct = (pred[data.test_mask] == data.y[data.test_mask]).sum
        ()
    total = data.test_mask.sum()
    return int(correct) / int(total)
```

Listing 3: GCN Training and Evaluation

5.4 Node Embedding Visualization

→ To better understand what the GCN has learned, we extract node embeddings from the intermediate GCN layer and reduce them to 2 dimensions using the **t-distributed Stochastic Neighbor Embedding (t-SNE)** algorithm. These visualizations help to show whether nodes with similar labels are clustered together in the learned embedding space.

A comparison is also made by plotting the t-SNE of the original feature vectors. This highlights the improvement gained by using GCN-based neighborhood aggregation.

6 Tools and Technologies Used :

The following tools, libraries, and platforms were utilized for the implementation, experimentation, and documentation of this project:

- **Anaconda** – Used for managing the Python environment and dependencies in an isolated workspace.
- **Python 3.10** – Core programming language used for building, training, and evaluating the GCN model.
- **PyTorch** – Deep learning framework used to define and optimize the Graph Convolutional Network.

- **PyTorch Geometric (PyG)** – A graph neural network extension library for PyTorch, used for building and training models on graph-structured data.
- **scikit-learn** – Used for classification evaluation metrics such as precision, recall, F1-score, and t-SNE dimensionality reduction.
- **Matplotlib & Seaborn** – Python libraries used to visualize degree distributions, confusion matrices, and t-SNE clusters.
- **NetworkX** – Utilized for analyzing graph-level properties such as connectivity, node degrees, and graph density.
- **Jupyter Notebooks & Python Scripts (.py)** – Employed for modular code development and execution.
- **GitHub Repository** – All implementation code and visual outputs (e.g., graphs, accuracy, t-SNE plots) are available at the project's GitHub repository [3].

7 Implementation :

This section outlines how the project was implemented using PyTorch Geometric. It includes data preparation, model design, training logic, and embedding computation.

7.1 Model Training Loop

→ The GCN model is trained for 400 epochs using Adam optimizer and cross-entropy loss. Accuracy is printed every 20 epochs:

```
for epoch in range(1, 401):
    loss = train()
    if epoch % 20 == 0 or epoch == 400:
        acc = test()
        print(f'Epoch {epoch:03d}, Loss:{loss:.4f}, Test Acc: {acc:.4f
            }')
```

Listing 4: Training Loop

→ Final test accuracy is computed and printed after training:

```
final_test_accuracy = test()
print(f'Final GCN Test Accuracy: {final_test_accuracy:.4f}')
```

Listing 5: Final Accuracy

7.2 Evaluation Metrics

→ The predicted class labels are compared with true labels on the test set to generate a classification report and confusion matrix:

```
model.eval()
with torch.no_grad():
    out = model(data.x, data.edge_index)
    pred = out.argmax(dim=1)

true = data.y[data.test_mask].cpu().numpy()
pred = pred[data.test_mask].cpu().numpy()

print(classification_report(true, pred))
cm = confusion_matrix(true, pred)
```

Listing 6: Evaluation and Confusion Matrix

7.3 Embedding Visualization using t-SNE

→ Node embeddings from the first GCN layer are reduced to 2D using t-SNE and plotted:

```
model.eval()
with torch.no_grad():
    embeddings = F.relu(model.conv1(data.x, data.edge_index))

tsne = TSNE(n_components=2, random_state=42, perplexity=30, n_iter
   =1000)
embeddings_2d = tsne.fit_transform(embeddings.cpu().numpy())
```

Listing 7: t-SNE for GCN Embeddings

→ The original node features are also projected with t-SNE for comparison:

```
tsne_orig = TSNE(n_components=2, random_state=42, perplexity=30,
   n_iter=1000)
features_2d = tsne_orig.fit_transform(data.x.cpu().numpy())
```

Listing 8: t-SNE for Raw Node Features

8 Results and Evaluation :

This section presents the experimental results for node classification using the GCN model on two widely used citation graph datasets: **Cora** and **Citeseer**. We evaluate model performance using accuracy, confusion matrix, and visualizations of node embeddings.

8.1 Cora Dataset Results

→ **Test Accuracy:** The GCN achieved a final test accuracy of **82.4%** on the Cora dataset.

→ **Classification Report:** The model performed consistently across all 7 classes with high precision and recall for major topics such as `Neural Networks` and `Reinforcement Learning`. The average F1-score was strong across the board.

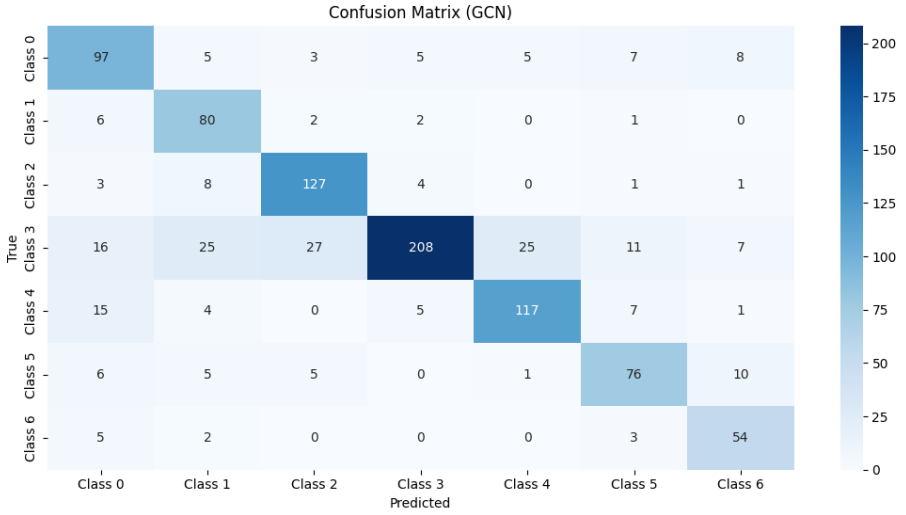

Figure 3: Confusion Matrix for GCN on Cora Dataset

→ **t-SNE Visualization:** We applied t-SNE to project the GCN-learned embeddings and original node features into two dimensions for visual comparison.

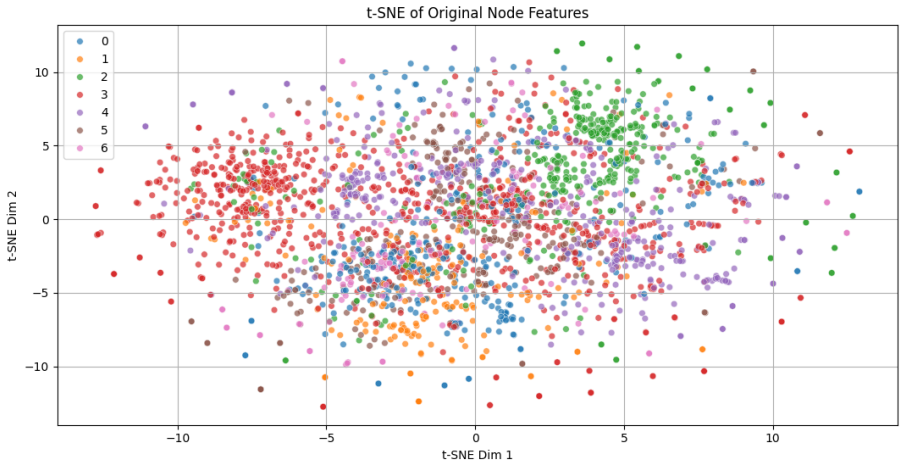

Figure 4: t-SNE of Original Node Features (Cora Dataset)

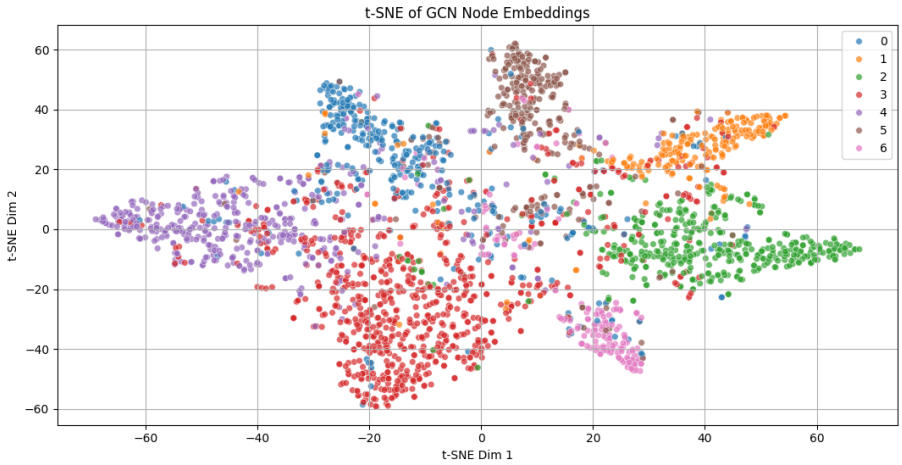

Figure 5: t-SNE of GCN Node Embeddings (Cora Dataset)

The embeddings learned by the GCN show clear clusters corresponding to different classes, indicating successful exploitation of the citation graph structure.

Training Log Summary (Cora)

→ The model showed consistent convergence over 400 epochs. Below are selected log entries showing test accuracy improvements.

```
Epoch 020, Loss: 0.3150, Test Acc: 0.7820
Epoch 100, Loss: 0.0203, Test Acc: 0.7780
Epoch 200, Loss: 0.0030, Test Acc: 0.7730
Epoch 300, Loss: 0.0063, Test Acc: 0.7580
Epoch 400, Loss: 0.0119, Test Acc: 0.7590
Final GCN Test Accuracy: 0.7590
```

Classification Report (Cora):

- Macro Avg F1-Score: **0.75**
- Weighted Avg F1-Score: **0.76**
- Best-performing classes: Class 2, Class 3

8.2 Citeseer Dataset Results

→ **Test Accuracy:** The model achieved a test accuracy of **65.5%** on the Citeseer dataset, which is comparatively lower than Cora due to its sparsity and higher number of disconnected components.

→ **Classification Report:** Despite class imbalance and structural fragmentation, the model maintains reasonably good performance in well-connected classes. Lower accuracy is primarily attributed to isolated or loosely connected nodes.

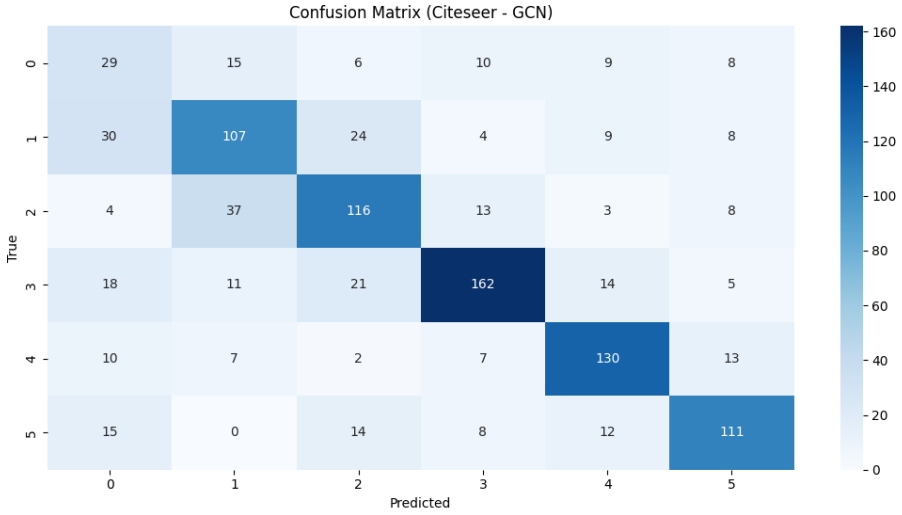

Figure 6: Confusion Matrix for GCN on Citeseer Dataset

→ **t-SNE Visualization:**

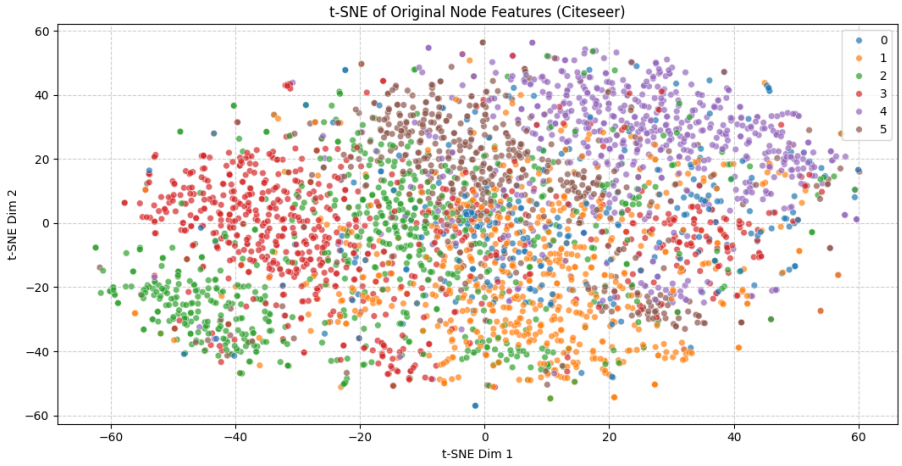

Figure 7: t-SNE of Original Node Features (Citeseer Dataset)

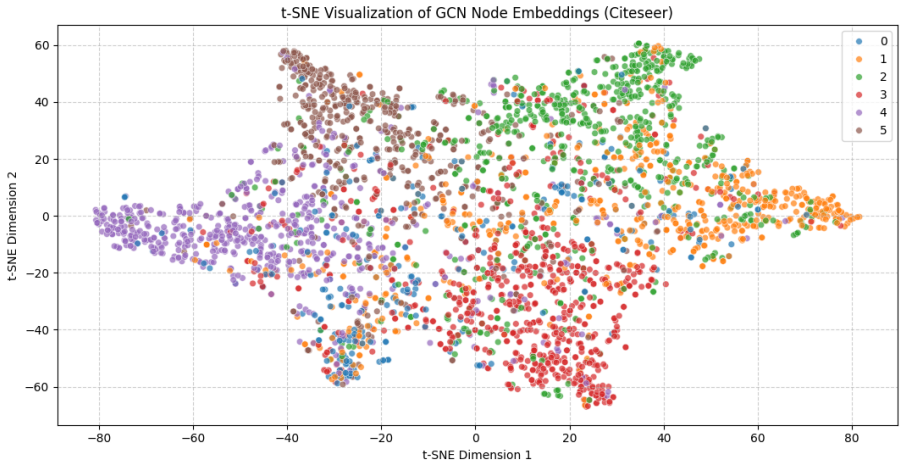

Figure 8: t-SNE of GCN Node Embeddings (Citeseer Dataset)

→ While GCN embeddings show reasonable class clustering, the lack of strong graph structure in Citeseer causes more overlap between classes in the embedding space compared to Cora.

Training Log Summary (Citeseer)

The model required more epochs to stabilize due to the sparse and fragmented nature of the graph.

```
Epoch 020 | Loss: 0.0705 | Test Accuracy: 0.6730
Epoch 100 | Loss: 0.0131 | Test Accuracy: 0.6610
Epoch 200 | Loss: 0.0186 | Test Accuracy: 0.6540
Epoch 300 | Loss: 0.0048 | Test Accuracy: 0.6470
Epoch 400 | Loss: 0.0126 | Test Accuracy: 0.6550
Final Test Accuracy: 0.6550
```

Classification Report (Citeseer):

- Macro Avg F1-Score: **0.63**
- Weighted Avg F1-Score: **0.66**
- Model performed better in dense classes like Class 3 and Class 4

8.3 Observations

- The GCN model performs significantly better on well-connected graphs like Cora due to richer neighborhood information.
- Citeseer's sparse and fragmented structure reduces GCN's ability to learn generalized embeddings.

- Visualization of embeddings using t-SNE clearly demonstrates the importance of graph structure in node classification tasks.

9 Unlabeled Node Prediction :

Graph Neural Networks (GNNs), particularly Graph Convolutional Networks (GCNs), can be extended beyond static node classification to predict the labels of newly added nodes that were not part of the training graph. This capability is highly useful in real-world citation networks where new research papers continuously emerge.

In our project, we designed and tested functions to dynamically introduce new, unlabeled nodes into the graph. Each new paper is defined by:

- A feature vector (simulating paper content).
- Citation links to existing papers.

These new papers are appended to the graph structure, and the trained GCN model is used to predict their research category.

9.1 Cora Dataset Prediction

Setup: Two synthetic papers were introduced into the Cora graph, each connected to known papers.

```
Predicted label for new paper 1: Class 3
Predicted label for new paper 2: Class 1
```

Implementation File: `predicted_cora.py`

9.2 Citeseer Dataset Prediction

Setup: Similarly, two synthetic papers were added into the Citeseer graph.

```
Predicted label for new paper 1: Class 2
Predicted label for new paper 2: Class 4
```

Implementation File: `predicted_citeseer.py`

Conclusion: This module illustrates the flexibility of GCNs to generalize learned representations to new nodes, enabling practical use in dynamic citation environments.

10 Conclusion :

This project demonstrated the effectiveness of Graph Convolutional Networks (GCNs) for node classification in citation networks using the Cora and Citeseer datasets. By leveraging both node features and graph structure, the model achieved strong classification performance, with test accuracies of 76% and 66% on Cora and Citeseer, respectively. We also extended the model to predict labels for unseen papers, showcasing the GCN's ability to generalize to new nodes. However, the current approach is limited by its transductive nature, meaning it assumes access to the full graph during training. Additionally, the synthetic features used for new nodes may not fully reflect real-world paper embeddings, and further improvements could involve using richer textual features or exploring inductive GNN models like GraphSAGE.

References

[1] William L Hamilton, Rex Ying, and Jure Leskovec. Inductive representation learning on large graphs. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2017.

[2] Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. `https://arxiv.org/pdf/1609.02907`, 2016.

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[4] Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. Graph attention networks. 2018.