Introduction To Geometric Deep Learning

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1 Introduction

This midterm evaluation report for the project "Geomtric deep learning" evaluates the student's progress and comprehension of Lecture 1 of Stanford University's "ML with Graphs" course, CS224W. This report's goal is to give a summary of the lecture's main ideas, personal development, and opportunities for growth.

2 Introduction to graphs ML and their representation

This topic introduces the concept of graphs and their representation using nodes (vertices) and edges (links). Graphs are a fundamental data structure used to model relationships and structures in various domains.

2.1 Why Graphs?

1.Show complex relationships and dependencies between entities.
2.Enable network analysis to understand connectivity and community structure.
3.Facilitate the development of graph algorithms for clustering and link prediction.
4.Serve as a natural representation for node and edge-level machine learning tasks.
5.Aid in visualizing large-scale networks, helping to extract meaningful insights.

2.2 Different types of graphs:

The lecture discusses a variety of graph types, including weighted, unweighted, directed, and undirected graphs. Undirected graphs lack directionally-directed edges, whereas directed graphs do. In weighted graphs, edges are given values to indicate their strength or significance.

2.3 Notions of nodes, edges, and attributes in graphs:

While edges (links) connect nodes (vertices) and represent relationships, nodes stand in for entities or elements. Both nodes and edges may be accompanied by features or attributes, adding more data for analysis.

2.4 Basics of graph visualization and network analysis:

Graph visualization involves representing the structure and patterns of a graph visually. It helps in exploring and understanding complex graph data. Network analysis focuses on studying the properties and behaviors of a network, such as identifying communities or detecting anomalies.

2.5 Graph properties: connectivity, density, and centrality measures:

- Connectivity measures determine the connectedness of a graph. Connected components are sets of nodes that can be reached from each other through a series of edges. Strongly connected components exist in directed graphs, where there is a directed path between any pair of nodes.

- Graph density quantifies the sparsity or connectedness of a graph by comparing the number of actual edges to the maximum possible edges.

- Centrality measures help identify important nodes in a graph. Degree centrality measures the number of edges connected to a node, while betweenness centrality quantifies the extent to which a node lies on the shortest paths between other nodes.

3 Applications Of Graphs in Real World

Many real-world data can be naturally represented as graphs, where nodes represent entities and links represent relationships or interactions between entities. Examples include social networks, citation networks, protein-protein interaction networks, and road networks. By learning node and link-level prediction features, we can effectively capture the underlying structure and dynamics of these graphs, enabling us to extract valuable insights and make predictions.

3.1 Node-level tasks and features

Node-level prediction focuses on predicting properties or labels associated with individual nodes in a graph. For example, in a social network, we might be interested in predicting the occupation, age group, or political affiliation of a user based on their interactions and attributes. By learning node-level prediction features, we can classify nodes into different categories or assign numerical values to them, which can be useful for various tasks such as targeted advertising, recommendation systems, and identifying anomalies.

4 Applications of Graphs in ML

4.1 Node-level ML Tasks: Protien folding

Protein folding is a node-level machine learning. It needs estimating a protein's 3D structure from its amino acid sequence. In a graph, amino acids are nodes, and machine learning techniques, such as graph neural networks (GNNs), learn patterns and features at the level of the individual amino acid to forecast folding patterns. It has implications for drug discovery and disease understanding.

4.2 Edge-level of graph ML

1- Recommender system

Recommender systems are one type of edge-level machine learning problem in ML with Graphs. They are designed to anticipate and recommend relevant goods to users based on their preferences and previous data. In a graph, edges reflect the connections between users and items. In order to provide customised suggestions, edge-level machine learning algorithms, including graph neural networks (GNNs), collect patterns and information from user-item interactions. Applications for recommender systems in e-commerce, content platforms, and customised marketing are numerous.

2- Drug side effects

Predicting and comprehending the negative effects of medications on patients is an example of an edge-level machine learning task in ML with Graphs. In a graph, the connections between medications and their adverse effects are shown as edges. To find possible adverse effects, edge-level machine learning algorithms, including graph neural networks (GNNs), learn patterns and features from drug-side effect correlations. These algorithms can help with drug development, enhance patient safety, and aid in the discovery of novel drug-target interactions by analysing the graph structure.

4.3 Subgraph- level ML tasks: Traffic prediction

Predicting traffic conditions and patterns at the level of subgraphs inside a road network is an example of a subgraph-level machine learning task in ML with Graphs. Localised regions or road segments within the wider network are represented by subgraphs. In order to predict traffic congestion, journey durations, or accident chances, machine learning algorithms, such as graph neural networks (GNNs), learn patterns and characteristics from the subgraph structure, historical traffic data, and numerous environmental parameters. These algorithms can help with real-time traffic management, route planning, and transportation infrastructure optimisation by looking at subgraphs.

5 Representing Graphs: Adjacency Matrix

Graphs can be represented in form of a matrix for operational and calculative purposes. Among the simplest of these matrices, $Aij = 1$ if there is a link between i^{th} and j^{th} nodes and $Aij = 0$ if no link is present. In this matrix, Aij represents a link from i^{th} node to j^{th} node. Order of these square matrices is same as total number of nodes in that graph.

It is worth noting that most real world networks are sparse. This implies most elements in adjacency matrix of graphs of these networks are zero. It can be understood from the fact that degree of a node in real network is way less that total number of nodes in that network.

6 Representation of Different Types of Graphs

Based on their own characteristics and properties, Different graphs can be represented in matrix form.

6.1 Directed and Undirected Graphs

As an undirected graph is a graph where the edges do not have a specific direction associated with them, the edges represent symmetric relationships between vertices. This means that if there is an edge between vertex A and vertex B, there is also an edge between vertex B and vertex A.

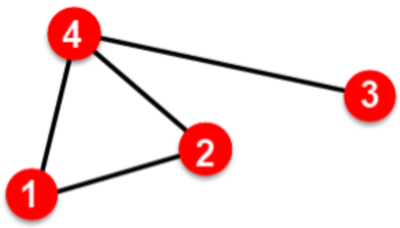


Figure 1: Example of Undirected Graph Representation

$$\begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$

It can be observed that the property of symmetry in graph is extended to it's matrix form. Furthermore, As directed graph (or digraph) is a graph where the edges have a specific direction associated with them, the edges represent asymmetric relationships between vertices. This means that if there is an edge from vertex A to vertex B, it does not necessarily imply the existence of an edge from vertex B to vertex A. The edges in a directed graph have a distinct source (starting vertex) and target (ending vertex). A similar

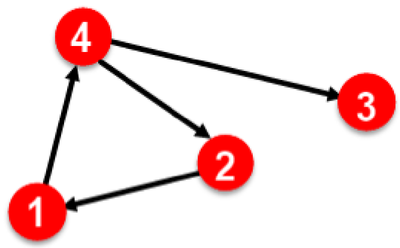


Figure 2: Example of Directed Graph Representation

$$\begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

observation can be made about asymmetry being extended to graph's matrix form.

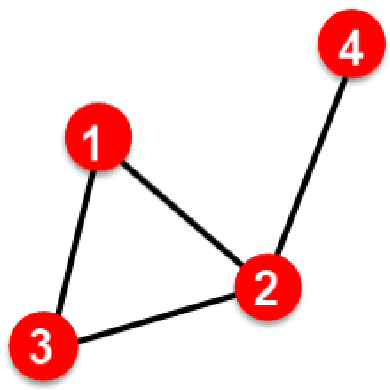
6.2 Weighted and Unweighted Graphs

In an unweighted graph, all edges have equal importance or weight. Each edge is represented as a connection between two vertices without any additional numerical value associated with it. Friendship and Hyperlink can be represented with this graph.

In a weighted graph, each edge has an associated weight or value. The edge weight represents a numerical measure of the importance, distance, cost, or any other property associated with the connection between two vertices. Road networks and social networks can be represented with these graphs.

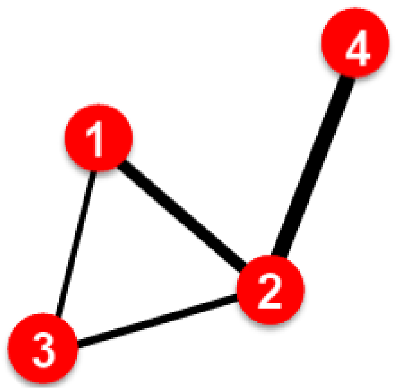
6.3 Self-edges (Self Loops)

A self-edge (or self-loop) is an edge that connects a vertex to itself. It represents a connection or relationship within a single vertex. It's matrix form is characterised by Aij not zero. Proteins and Hyperlinks are represented by these graphs.



$$\begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

Figure 3: Example of Unweighted Graph Representation



$$\begin{bmatrix} 0 & 2 & 0.5 & 1 \\ 2 & 0 & 1 & 4 \\ 0.5 & 1 & 0 & 0 \\ 0 & 4 & 0 & 0 \end{bmatrix}$$

Figure 4: Example of weighted Graph Representation

6.4 Multigraphs

A multigraph is a type of graph that allows multiple edges between pairs of vertices. Unlike simple graphs, where only one edge can exist between any two vertices, multigraphs permit multiple parallel edges. The multiple edges can have different attributes, such as different weights, colors, or meanings.

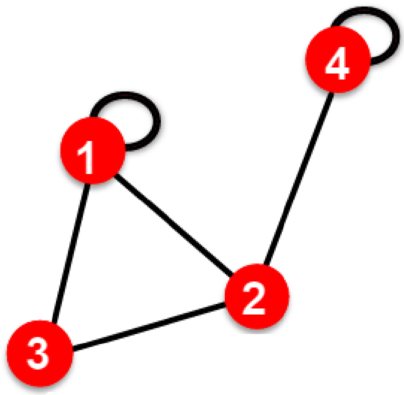
7 Connectivity

7.1 Undirected Graphs

These are of 2 types based on connectivity, connected and disconnected.
In a Connected graph, one can always find a path to join any two of it's vertices. Contrary to this, A disconnected graph is made up of two or more connected components. While representing these graphs, The adjacency matrix of a network with several components can be written in a block-diagonal form, so that nonzero elements are confined to squares, with all other elements being zero.

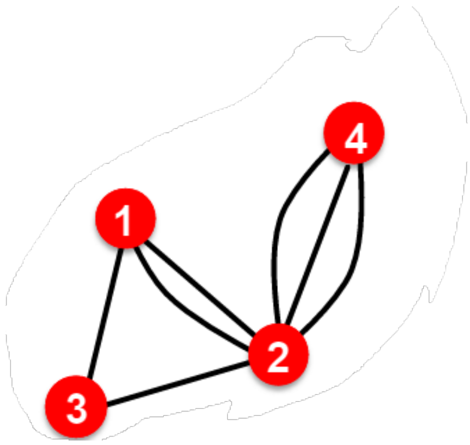
7.2 Directed Graphs

These are of 2 types based on connectivity, strongly-connected and weakly-connected.
A strongly-Connected graph has a path from each node to every other node and vice versa. A weakly-connected graph, on the other hand, is connected if we disregard the edge directions.
In such graphs, Strongly connected components (SCCs) can also be identified where in a particular component of the graph is strongly connected. But it is worth noting that not every node is part of a nontrivial strongly connected component. Through these components we can defines In-component and Ou-component nodes. In



$$\begin{bmatrix} 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$$

Figure 5: Example of Self Looped Graph Representation



$$\begin{bmatrix} 0 & 2 & 1 & 0 \\ 2 & 0 & 1 & 3 \\ 1 & 1 & 0 & 0 \\ 0 & 3 & 0 & 0 \end{bmatrix}$$

Figure 6: Example of Multigraph Representation

component nodes are those which can reach the SCC whereas Out-component nodes are those which can be reached from the SCC. In Example below E and G is In-component while D and F are out component.

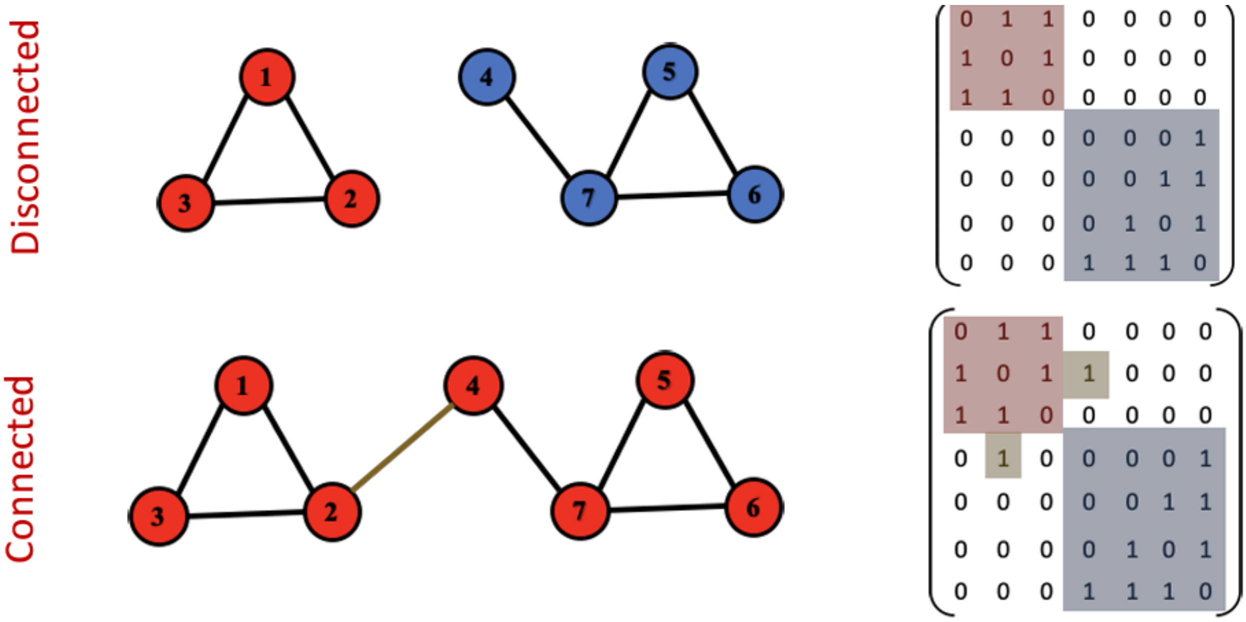


Figure 7: Connectivity of Undirected Graphs

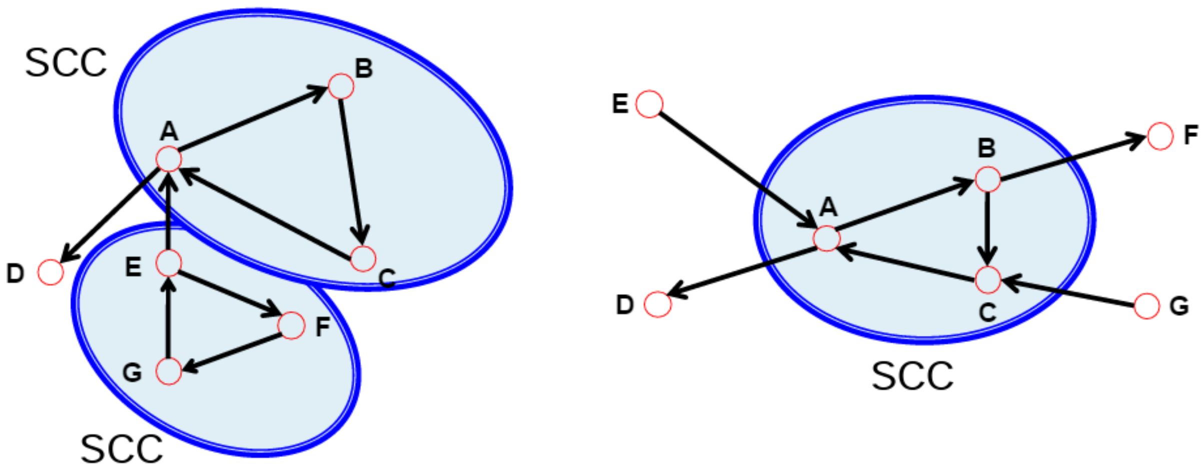


Figure 8: Strongly Connected Components in an Directed Graph

8 Implemenation

In this section, we discuss our assignment which focuses on graph creation using PyG.

8.1 Section-1: Graph Creation

8.1.1 Creating the following graph in PyG. The numbers inside the squares are both the ID and the values stored in the notes.

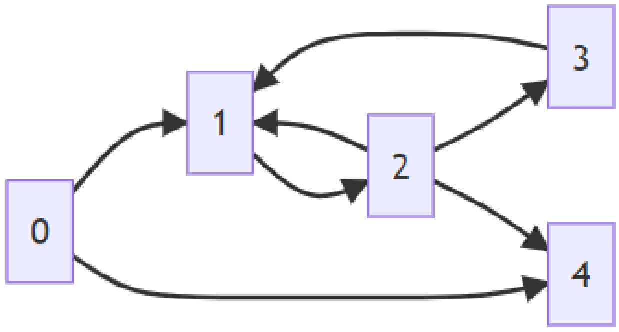


Figure 9: Graph

In here, we are trying to implement a specific directed graph in PyG. The graph consists of nodes with ID and values stored in them.

```
import torch
from torch_geometric.data import Data

# Define the edge indices
edge_index = torch.tensor([[0, 0, 1, 2, 2, 2, 3],
                           [1, 4, 2, 1, 3, 4, 1]], dtype=torch.long)

# Define the node features
x = torch.tensor([[0], [1], [2], [3], [4]], dtype=torch.float)

# Create the PyG Data object
data = Data(x=x, edge_index=edge_index)
```

In the above code, the `edge_index` tensor defines the edge connections between nodes, and the `x` tensor represents the node features. Finally, the `Data` object is created, encapsulating the graph structure and node features.

8.1.2 Complete the code to visualise the graph using the utilities module of PyG

We write the code to visualize the graph using the utilities module of PyG to create a NetworkX `Graph` object. The `to_networkx` function is used to convert the PyG `Data` object to a NetworkX `Graph` object. The resulting `Graph` object can be passed to the `visualize_graph` helper function for visualization.

The provided code snippet demonstrates how to visualize the graph using the `visualize_graph` function with the NetworkX `Graph` object.

```
from torch_geometric.utils import to_networkx
import networkx as nx
import matplotlib.pyplot as plt

# Convert PyG Data object to NetworkX Graph object
G = nx.DiGraph(to_networkx(data))

# Helper function for visualization
def visualize_graph(G):
    plt.figure(figsize=(7,7))
    plt.xticks([])
```

```
    plt.yticks([])
    nx.draw_networkx(G, pos=nx.spring_layout(G, seed=42), with_labels=True, cmap="Set3")
    plt.show()

# Visualize the graph using the visualize_graph function
visualize_graph(G)
```

The above code converts the PyG `Data` object to a NetworkX `Graph` object using the `to_networkx` function. The resulting `Graph` object is then passed to the `visualize_graph` function for visualization.

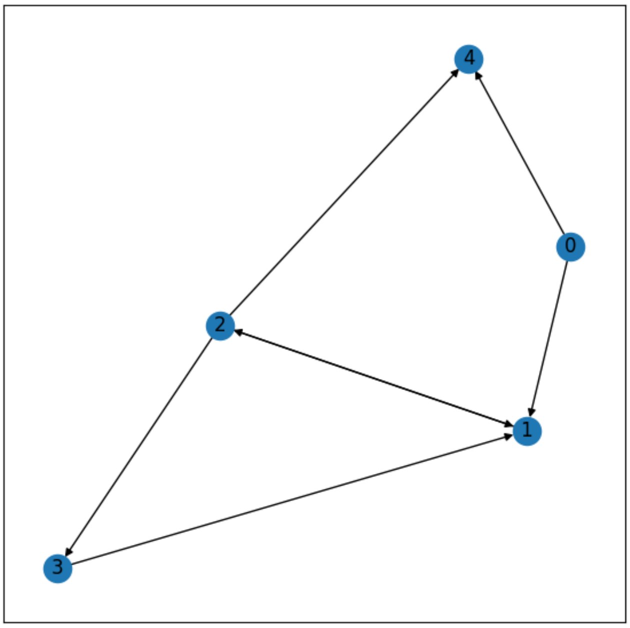


Figure 10: Output Graph

The resulting graph, as shown in Figure 10, matches the specified graph in the question.

8.1.3 Modifying existing graph

We attempt to modify the previously created graph by adding new nodes and edges. The modifications include adding a node with ID 5 and creating edges between specific nodes. The provided code snippet demonstrates how to make these modifications to the NetworkX `Graph` object.

```
# Add nodes and edges to the graph
G.add_edge(1, 5)
G.add_edge(5, 0)
G.add_edge(5, 2)
G.add_edge(2, 5)

# Visualize the modified graph
visualize_graph(G)
```

The above code adds a node with ID 5 and creates edges between nodes 1 and 5, 5 and 0, and 2 and 5. These modifications update the graph structure accordingly. Finally, the modified graph can be visualized using the `visualize_graph` function.

The resulting graph, as shown in Figure 11, matches the specified graph in the question.

8.2 Section-2: Graph Properties and Manipulation

8.2.1 Basic properties of a given graph

The properties include the number of nodes, edges, node features, and directedness of the graph, to be returned as the tuple:

`(#nodes, #edges, #features, directedness)`

The function `get_basic_chars` is implemented as follows:

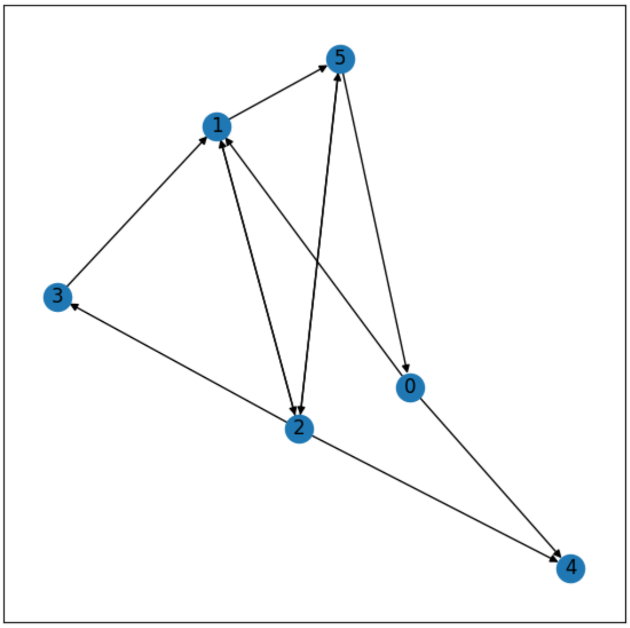


Figure 11: Output Graph

```
def get_basic_chars(dataset):
    nodes = dataset.num_nodes
    edges = dataset.num_edges
    features = dataset.num_node_features
    directedness = dataset.is_directed()
    chars = (nodes, edges, features, directedness)
    return chars

# Call the function on the 'mutag' graph
get_basic_chars(mutag)
```

The `get_basic_chars` function takes a PyG `Dataset` object as input and extracts the required properties using the provided PyG functions. The properties are then returned as a tuple: `(42, 162, 3, False)`.

When called on the 'mutag' graph, the function returns the following output: `(42, 162, 3, False)`. This indicates that the 'mutag' graph has 42 nodes, 162 edges, 3 node features, and is not directed.

8.3 Self Loops and Isolated Nodes

We need to determine whether the graph has any self loops or isolated nodes. The code snippet below demonstrates this:

```
def addn_props(dataset):
    # Check for self loops
    self_obsessed = dataset.has_self_loops()

    # Check for isolated nodes
    loners = dataset.has_isolated_nodes()

    return (self_obsessed, loners)

addn_props = addn_props(mutag)
print(f'Does␣this␣graph␣have␣self␣loops?␣{addn_props[0]}')
print(f'Does␣this␣graph␣have␣isolated␣nodes?␣{addn_props[1]}')
```

The code defines the `addn_props` function, which takes a dataset as input. It uses the `has_self_loops()` and `has_isolated_nodes()` functions to check for self loops and isolated nodes in the dataset, respectively. The results are stored in the `self_obsessed` and `loners` variables. Finally, the results are printed.

The output will be:

```
Does this graph have self loops? False
Does this graph have isolated nodes? False
```

8.3.1 Average Degree of the network

We compute the average degree of the network, rounded to the nearest integer. The code snippet below demonstrates this:

```
def avg_degree(G):
    sum = 0
    for node in G.nodes():
        sum += G.degree(node)
    avg_deg = round(sum / len(G.nodes()))
    return avg_deg

avg_deg = avg_degree(G)
print(f'Average degree of MUTAG is {avg_deg}')
```

The code defines the `avg_degree` function, which takes a graph `G` as input. It iterates over all the nodes in the graph and accumulates their degrees. The average degree is then calculated by dividing the sum of degrees by the number of nodes and rounding it to the nearest integer. Finally, the average degree is printed.

The output will be:

```
Average degree of MUTAG is 4
```

8.3.2 Splitting Dataset

We implement splitting the dataset into train-validation-test sets in a specific ratio.However, Since the dataset is split into a different train-val-test ratio already, we'll have to combine them and resplit them again to get the desired split. The code snippet below demonstrates this:

```
import random

tot_ind = list(range(len(mutag_datasets)))
random.shuffle(tot_ind)

train_split = int(0.75 * len(tot_ind))
val_split = int(0.90 * len(tot_ind))

train, val, test = mutag_datasets[tot_ind[:train_split]], mutag_datasets[tot_ind[train_split
    ↪ :val_split]], mutag_datasets[tot_ind[val_split:]]
```

The code first imports the `random` library for shuffling the dataset indices. It creates a list of indices (`tot_ind`) representing the dataset. The list is shuffled using `random.shuffle()`. Then, the indices are used to split the dataset into three sets: training, validation, and testing. The splitting is based on the provided ratios: 75% for training, 15% for validation, and 10% for testing. The resulting sets are stored in the `train`, `val`, and `test` variables.

The output will be:

```
Train set size: 834
Validation set size: 167
Test set size: 112
```

8.3.3 Small-Worldness Coefficients

We calculate the sigma and omega coefficients for small-worldness using two different methods: the direct method (using the built-in functions) and the manual method (calculating the required values manually). The code snippet below demonstrates this:

```
import time

# Direct method
start = time.time()
sigma = nx.sigma(G)
```

```
omega = nx.omega(G)
direct_time = time.time() - start

# Manual method
def calc_sig_omg(G):
    start = time.time()

    c_c = nx.clustering(G)
    c = sum(c_c.values()) / len(c_c)
    l = nx.average_shortest_path_length(G)
    R = nx.erdos_renyi_graph(len(G), nx.density(G))
    while not nx.is_connected(R):
        R = nx.erdos_renyi_graph(len(G), nx.density(G))
    L = nx.watts_strogatz_graph(len(G), int(c * len(G)), 0)
    c_L = sum(nx.clustering(L).values()) / len(nx.clustering(L))
    c_R = sum(nx.clustering(R).values()) / len(nx.clustering(R))
    l_L = nx.average_shortest_path_length(L)
    l_R = nx.average_shortest_path_length(R)
    sig = (c / c_R) / (l / l_R)
    omg = (l_R / l) - (c / c_L)
    man_time = time.time() - start

    return (sig, omg, man_time)

sig, omg, man_time = calc_sig_omg(G)

print(f'Direct␣Sigma␣Coefficient:␣{sigma}')
print(f'Direct␣Omega␣Coefficient:␣{omega}')
print(f'Time␣for␣Direct␣Method:␣{direct_time}')
print(f'Conv␣Sigma␣Coefficient:␣{sig}')
print(f'Conv␣Omega␣Coefficient:␣{omg}')
print(f'Time␣for␣Conv␣Method:␣{man_time}')
```

The code first imports the `time` library for measuring the execution time. Then, it calculates the sigma and omega coefficients using two methods: the direct method (using the built-in functions `nx.sigma()` and `nx.omega()`) and the manual method (calculating the required values manually). The execution time for each method is measured, and the results are printed.

The sigma and omega coefficients for small-worldness are calculated using the random shuffled graph (R) and lattice graph (L). Here is an explanation for why these specific types of graphs are used:

1. Random shuffled graph (R): The random shuffled graph is generated using the Erdős-Rényi model. This model randomly connects pairs of nodes in the graph with a given probability. It is used to create a random graph that serves as a reference for comparison. The purpose of using R is to evaluate the randomness and clustering of the original graph (G) by comparing its clustering coefficient (c) and average shortest path length (l) with those of R.

2. Lattice graph (L): The lattice graph is generated using the Watts-Strogatz model. This model starts with a regular lattice structure where each node is connected to its nearest neighbors. Then, a small fraction of edges are randomly rewired. The rewiring process introduces randomness while preserving the local clustering property. The purpose of using L is to evaluate the clustering coefficient (c_L) and average shortest path length (l_L) of a graph with high local clustering and low global clustering.

By comparing the clustering coefficients and average shortest path lengths of G, R, and L, the sigma and omega coefficients are calculated. The sigma coefficient compares the clustering of G with that of R, while the omega coefficient compares the clustering of G with that of L. These coefficients provide a measure of how close G is to being a small-world network.

Using R and L allows for a comparative analysis of G's clustering and average path lengths against random and highly clustered structures. This comparison helps determine whether G exhibits small-world characteristics, such as high clustering and short average path lengths, which are indicative of efficient information transfer and characteristic of small-world networks.

The output will be:

```
Direct Sigma Coefficient: 2.0694165696330655
Direct Omega Coefficient: -0.4749945875730678
```

```
Time for Direct Method: 104.85231828689575
Conv Sigma Coefficient: 3.454863430265677
Conv Omega Coefficient: 0.1817438839575665
Time for Conv Method: 0.008679628372192383
```

8.4 Clustering Coefficient

In this section, we explore more about the clustering coefficient and its relation to node degrees and the adjacency matrix using wedges(ordered triplet of edges sharing exactly one common node).

8.4.1 Local clustering coefficient

We have derived an expression for local clustering coefficient C_i using node degrees k_i and adjacency matrix A.
$C_i = \frac{1}{k_i(k_i-1)} \sum_{j,k} A_{ij} A_{jk} A_{ki}$
The term $A_{ij} A_{jk} A_{ki}$ gives 1 only when edges exist between i, j and k nodes thus its sum gives number of links between neighbours of i.

8.4.2 Global Clustering Coefficient

Assuming network has finite nodes, we have derived the expression for global clustering coefficient C
$C = \frac{\sum_{i \neq j \neq k} A_{ij} A_{jk} A_{ki}}{\sum_i k_i(k_i-1)}$.
$\sum_i k_i(k_i - 1)$ gives the total number of possible triplets of nodes and $k_i = \sum_j A_{ij}$ is the degree of node i and $C = 0$ when denominator is 0.

8.4.3 Back-in-2 coefficient

We have defined a back-in-2 coefficient $(Bi_2(i))$ as fraction of wedges headed at i that are closed and derived an expression for it .
$Bi_2(i) = \frac{\sum_{i \neq j \neq k} A_{ij} A_{jk} A_{ki}}{\sum_{j \neq k} A_{ij} A_{ki}}$

8.5 Conclusion

This assignment has provided hands-on experience in creating, manipulating, and analyzing graphs using PyG and NetworkX. The tasks covered graph creation, visualization, and extraction of basic graph properties. These concepts are fundamental in the field of Geometric Deep Learning and form the building blocks for more advanced graph-based algorithms and models. It also introduces us to the concept of small world graphs and how to calculate small worldness of a given graph. Small world networks have extensive applications in sociology, earth sciences and computing.