

# Concepts and Techniques of Graph Neural Networks

Vinod Kumar

*Koneru Lakshmaiah Education Foundation (Deemed), India*

Dharmendra Singh Rajput

*VIT University, India*

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Communication, India*

The vertices, which are also known as nodes or points, and the edges, which are responsible for connecting the vertices to one another, are the two primary components that make up a graph. Graph theory is the mathematical study of graphs, which are structures that are used to depict relations between items by making use of a pairwise relationship between them. Graphs can be thought of as a visual representation of a mathematical equation. The principles of graph theory will be covered in this chapter.

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*Sougatamoy Biswas, National Institute of Technology, Rourkela, India*

Graph neural network (GNN) is an emerging field in deep learning. Graphs have more expressive power than any other data structure. Graph neural network is one of the application areas of deep learning, and it has applications in different domains where traditional convolutional neural networks can't give the desired result. Graphs are basically connections of nodes through the edges. In the area of recommendation systems, image processing and fraud detection are some of the few application areas of graph neural networks. As graphs are moveable and mobile in nature, they are more flexible to apply in these domains. GNN deals with these types of problems more effectively than a convolution neural network. To apply GNN to a specific problem domain, data needs to be converted into a graphical format, and then neural network operations can be executed. The main feature of GNN is to inherit information from its neighborhood. This is called graph embedding. This chapter describes basic GNN architecture, GNN advantage over CNN, and its application in different domains.

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*Ganga Devi S. V. S., Madanapalle Institute of Technology and Science, India*

Deep learning on graphs is an upcoming area of study. This chapter provides an introduction to graph neural networks (GNNs), a type of neural network that is designed to process data represented in the form of graphs. First, it summarizes the explanation of deep learning on graphs. The fundamental concepts of graph neural networks, as well as GNN theories, are then explained. In this chapter, different types of graph neural network (GNN) are also explained. At the end, the applications of graph neural network where GNN is used and for what purpose it is going to be used are explained. This also explores the various applications of GNNs in fields such as social network analysis, recommendation systems, drug discovery, computer vision, and natural language processing. With the increasing prevalence of graph data, GNNs are becoming increasingly important and will likely continue to play a significant role in many fields in the future.

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*Gotam Singh Lalotra, Government Degree College, Basohli, India*

*Ashok Sharma, University of Jammu, India*

*Barun Kumar Bhatti, Government Degree College for Women, Kathua, India*

*Suresh Singh, GGM Science College, Jammu, India*

Graph neural networks have recently come to the fore as the top machine learning architecture for supervised learning using graph and relational data. An overview of GNNs for graph classification (i.e., GNNs that learn a graph level output) is provided in this chapter as pooling layers, or layers that learn graph-level representations from node-level representations, are essential elements for successful graph classification because GNNs compute node-level representations. Hence, the authors give a thorough overview of pooling layers. The constraints of GNNs for graph categorization are further discussed, along with developments made in overcoming them. Finally, they review some GNN applications for graph classification and give an overview of benchmark datasets for empirical analysis.

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*Himanshu Verma, B.K. Birla Institute of Engineering and Technology, Pilani, India*

*Yogesh Kumar Sharma, Koneru Lakshmaiah Education Foundation (Deemed), India*

Graph neural networks (GNNs) are a useful tool for analyzing graph-based data in areas like social networks, molecular chemistry, and recommendation systems. Adversarial attacks on GNNs include introducing malicious perturbations that manipulate the model's predictions without being detected. These attacks can be structural or feature-based depending on whether the attacker modifies the graph's topology or node/edge features. To defend against adversarial attacks, researchers have proposed countermeasures like robust training, adversarial training, and defense mechanisms that identify and correct adversarial examples. These methods aim to improve the model's generalization capabilities, enforce regularization, and incorporate defense mechanisms into the model architecture to improve its robustness against attacks. This chapter offers an overview of recent advances in adversarial attacks on GNNs, including attack methods, evaluation metrics, and their impact on model performance.

## Chapter 6

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*R. Soujanya, Gokaraju Rangaraju Institute of Engineering and Technology, Hyderabad, India*

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*Manish Manish Maheshwari, Makhanlal Chaturvedi National University of Journalism and Communication, Bhopal, India*

*Divya Prakash Shrivastava, Higher Colleges of Technology, Dubai, UAE*

Graph attention networks, also known as GATs, are a specific kind of neural network design that can function on input that is arranged as a graph. These networks make use of masked self-attentional layers in order to compensate for the shortcomings that were present in prior approaches that were based on graph convolutions. The main advantage of GAT is its ability to model the dependencies between nodes in a graph, while also allowing for different weights to be assigned to different edges in the graph. GAT is able to capture both local and global information in a graph. Local information refers to the information surrounding each node, while global information refers to the information about the entire graph. This is achieved through the use of attention mechanisms, which allow the network to selectively focus on certain nodes and edges while ignoring others. It also has scalability, interpretability, flexibility characteristics. This chapter discusses the fundamental concepts in graph attention networks.

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Social networks are complex systems that require specialized techniques to analyze and understand their structure and dynamics. One important task in social network analysis is link prediction, which involves predicting the likelihood of a new link forming between two nodes in the network. Graph convolutional neural networks (GCNNs) have recently emerged as a powerful approach for link prediction, leveraging the graph structure and node features to learn effective representations and predict links between nodes. This chapter provides an overview of recent advances in GCNNs for link prediction in social networks, including various GCNN architectures, feature engineering techniques, and evaluation metrics. It discusses the challenges and opportunities in applying GCNNs to social network analysis, such as dealing with sparsity and heterogeneity in the data and leveraging multi-modal and temporal information. Moreover, this also provides reviews of several applications of GCNNs for link prediction in social networks.

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*Gayathri Dhara, SRM University, India*

*Ravi Kant Kumar, SRM University, India*

GNNs (graph neural networks) are deep learning algorithms that operate on graphs. A graph's unique ability to capture structural relationships among data gives insight into more information rather than by analyzing data in isolation. GNNs have numerous applications in different areas, including computer vision. In this chapter, the authors want to investigate the application of graph neural networks (GNNs) to common computer vision problems, specifically on visual saliency, salient object detection, and

co-saliency. A thorough overview of numerous visual saliency problems that have been resolved using graph neural networks are studied in this chapter. The different research approaches that used GNN to find saliency and co-saliency between objects are also analyzed.

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*Ram Kumar, Lovely Professional University, India*

*Monica Sankat, Lovely Professional University, India*

The chapter consists of the application of GNN with all applied fundamentals in different fields of application. Firstly, the discussion will be about the graph using graph theory connection to the mathematical aspect. Secondly, the basis of the data set will be for forecasting and predictive analysis, application, and fundamental concepts, which will help in decision making regarding the different unsolved problems. Third, knowledge about the models of the graph neural network with the examples will be a very important part of the chapter. This chapter is useful for fulfilling the research gap in the field of some forecasting models using graph neural networks with the application of machine learning on data analysis with a large number of examples.

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*Ab Qayoom Sofi, Lovely Professional University, India*

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The lifestyle of people across the globe has become fast and faulty, which has resulted in a highly stressful life full of anxiety and depression. People's habits have become very unhealthy, which has led to huge rise in several Non-Communicable diseases (NCDs) or lifestyle disorders like diabetes, hypertension, cardio vascular diseases, mental health issues, etc. The heart disease is still the biggest cause of mortality in the world. It is spreading at an alarming rate due to bad lifestyles, consumption of junk food, smoking, drinking, and lack of awareness and alertness. These lifestyle disorders are spreading at an alarming rate and are spreading from epidemic to a pandemic. These, besides other health consequences, have serious social and economic implications for the individual and for the country. These conditions have multiple dimensions and can be controlled and prevented if diagnosed and treated in time by improving the overall personality of an individual with the help of technology and self-management.



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Predicting student performance becomes tougher thanks to the big volume of information in educational databases. Currently, in many regions, the shortage of existing system to investigate and monitor the coded progress and performance isn't being addressed. First, the study on existing prediction methods remains insufficient to spot the foremost suitable methods for predicting the performance of scholars in many institutions. Second is because of the shortage of investigations on the factors affecting student achievements particularly courses within specified context. Therefore, a systematic literature review on predicting student performance by using data processing techniques is proposed to enhance student achievements. The objective of this work is to supply an outline on the info techniques to predict student performance. Previous studies have extensively reported on optimizing performance predictions to highlight risky students and promote the achievement of good students. There are also contributions that overlap with various research fields.

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*Parveen Kumar, Chandigarh University, India*

*Vinay Bhatia, Chandigarh Engineering College, India*

*Ankur Singhal, Chandigarh Engineering College, India*

Graph data, which often includes a richness of relational information, are used in a vast variety of instructional puzzles these days. Modelling physics systems, detecting fake news on social media, gaining an understanding of molecular fingerprints, predicting protein interfaces, and categorising illnesses all need graph input models. Reasoning on extracted structures, such as phrase dependency trees and picture scene graphs, is essential research that is necessary for other domains, such as learning from non-structural data such as texts and photos. These types of structures include phrase dependency trees and image scene graphs. Graph reasoning models are used for this kind of investigation. GNNs have the ability to express the dependence of a graph via the use of message forwarding between graph nodes. Graph convolutional networks (GCN), graph attention networks (GAT), and graph recurrent networks (GRN) have all shown improved performance in response to a range of deep learning challenges over the course of the last few years.

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*Jayanti Mehra, Lakshmi Narain College of Technology, Bhopal, India*

*Neelu Singh, Lakshmi Narain College of Technology, Bhopal, India*

Face recognition is a process by which the identity of a person is determined from the face images stored in a face database. Face recognition is one of the most successful applications of image analysis. In the present scenario, face recognition plays a major role in commercial and law enforcement applications, such as surveillance system, passport, security, personal information accesses, human machine interaction, etc. At present, very reliable methods of biometric personal identification exist. In face recognition, a feature vector usually represents the salient characteristics that best describe a face image. However, these characteristics vary quite substantially while looking into a face image from different directions. This chapter addresses this issue by means of image fusion and presents a comprehensive study of different image fusion techniques for face recognition. Image fusion is done between the original captured image and its true/partial diagonal images.

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## Foreword

In recent years, Graph Neural Networks (GNNs) have emerged as a powerful tool for analyzing and processing graph-structured data. GNNs are a type of deep learning model that operates directly on graphs, allowing them to capture complex relationships and dependencies between nodes in a graph.

The field of GNNs is rapidly evolving, with new models and techniques being proposed on a regular basis. In this book, “Concepts and Techniques of Graph Neural Networks,” the authors provide a comprehensive introduction to the fundamental concepts and techniques of GNNs.

Starting with an overview of the basic concepts of graph theory and deep learning, the book delves into the core principles of GNNs, such as message passing, graph convolutional networks, and attention mechanisms. The authors then cover advanced topics such as graph attention networks, graph transformers, and graph adversarial training.

Throughout the book, the authors provide clear explanations and intuitive examples to help readers understand the underlying concepts and techniques of GNNs. The book also includes practical applications of GNNs in various domains, including social networks, chemistry, and computer vision.

The field of GNN continues to evolve very quickly, but this book is a quick way to learn the basic ideas and understand where the field is now. I thought it was very interesting and helpful, and I think you will too. Whether you are a researcher, practitioner, or student interested in learning about GNNs, this book will serve as an invaluable resource. The authors have done an excellent job of providing a thorough and accessible introduction to this exciting field, and I highly recommend this book to anyone interested in exploring the power of GNNs.

*Kamal Raj Pardasani*

*Department of Mathematics, Maulana Azad National Institute of Technology, Bhopal, India*

## Preface

Graph Neural Networks, also known as GNNs, have seen a meteoric rise in popularity over the past few years due to its capacity to analyse data that is shown in the form of graphs. GNNs have been put to use in a broad variety of industries, including social network research, the search for new drugs, recommender systems, and traffic prediction, to mention just a few examples. GNNs are becoming increasingly popular, which has resulted in an increased interest in the issue among scholars and practitioners who are interested in better comprehending the fundamental ideas and procedures that underpin GNNs. The book “Concepts and Techniques of Graph Neural Networks” is a reference to the concepts and procedures that are utilised in Graph Neural Networks (GNNs). GNNs have developed as an effective method for modelling complicated structured data, such as social networks, protein structures, and traffic patterns, among other applications. Applications have been identified for them in a broad variety of domains, such as drug discovery, computer vision, natural language processing, and recommender systems. GNNs are especially helpful for solving situations in which the data is modelled as a graph, in which the nodes of the graph represent entities and the edges reflect the relationships between those entities. Because GNNs are able to perform reasoning and inference by utilising the graph structure, they are ideally suited for solving problems in which the relationships between the entities are of primary significance. Today, research into GNNs is a field that is expanding at a rapid rate, and new ideas and methods are being developed on a consistent basis. This is an interdisciplinary area that draws on concepts from a variety of different fields, including computer science, mathematics, and statistics, among others. The relevance of GNNs is anticipated to expand as the amount of structured data continues to grow, which makes the ideas and approaches for GNNs an essential topic of research in the world as it exists today. GNNs are able to accomplish tasks such as node classification, link prediction, and graph classification by employing a mix of node and edge attributes. This allows the information to be propagated throughout the graph as the network is traversed. The fundamental concept underlying GNNs is that they should take advantage of the local connection patterns of the graph to extract relational information and then use this knowledge to the task of making predictions. Moreover, GNNs are able to handle large-scale, complicated graphs that contain millions or even billions of nodes and edges, which is one of the primary advantages of using these types of networks. GNNs also have the potential to overcome some of the difficulties that have arisen as a result of the increasing availability of graph-structured data in the world as it exists today. Large-scale graphs are frequently used to illustrate the intricacies of the interactions that exist between the many entities involved in a variety of areas, such as social networks, online markets, and transportation systems, to name just a few examples. Researchers and practitioners may construct models for analysing these graphs that are more accurate, scalable, and interpretable by utilising the capabilities of GNNs. These models will allow for the extraction of relevant insights. This book on “Concepts and

Techniques of Graph Neural Networks” aims to provide a comprehensive resource for anyone interested in understanding GNNs. The book covers both fundamental concepts and recent advances in the field, making it accessible to both beginners and experienced practitioners.

Several prominent researchers and practitioners in the fields of AI, ML, and graph mining contributed to the book’s 13 chapters. The book is organized in a logical progression from basic concepts to the corresponding technological solutions. The book’s material is structured as follows:

**Chapter 1:** This talks about basic and very important key terms related to graphs, such as graph and its different types, nodes, edges, degree of a graph, adjacency matrix, modelling of graphs, graph embedding, etc. Overall, this chapter is about the basics of graph theory and graphs for graph neural networks.

**Chapter 2:** This chapter talks about the Graph Neural Network and its design, the Graph Embedding Process, and the benefits of Graph Neural Networks over Graph Convolutional Networks. It also talks about the problems and new changes in GNN, as well as how it can be used in real life.

**Chapter 3:** This introduces Graph Neural Networks (GNNs) by outlining graph deep learning, GNN theories, general principles, and GNN types. GNN apps were described at the end, and GNN applications were also looked at.

**Chapter 4:** This gives a review of GNNs and how they can be used to classify graphs. It also talks about some of the problems and limits of GNNs and how they can be used in different ways to classify graphs. In addition, it gives an overview of standard datasets that can be used for empirical study.

**Chapter 5:** This chapter gives an overview of recent improvements in adversarial attacks on GNNs, including attack methods, evaluation measures, and how they affect model performance.

**Chapter 6:** This chapter talks about the basic ideas behind graph attention networks (GAT), including how they are put together. It also goes into more detail about how normal GCN and GAT are different. In addition, it shows how GAT can be used in important ways in the real world.

**Chapter 7:** This is about Graph Convolutional Neural Networks for Link Prediction in Social Networks. The GCNN design for link detection is covered. This shows how the social network data for GCNN was prepared before it was used.

**Chapter 8:** The writers want to look at how graph neural networks (GNNs) can be used to solve common computer vision problems, such as visual saliency, salient object recognition, and co-saliency. In this chapter, we look at how graph neural networks have been used to solve a number of problems with visual saliency. Also looked at are the different study methods that used GNN to find salience and co-salience between items.

**Chapter 9:** This chapter talks about the useful study gaps in the area of forecasting models that use Graph Neural Networks (GNN) and machine learning. This includes trial data analysis with different examples. Two case studies are also included to help you understand how GNN applications work.

**Chapter 10:** This chapter shows how Graph Neural Networks can be used in m-health to track diseases in people. It also says that health information technology (HIT) that is digital is the way of the future.

**Chapter 11:** This chapter looks at how Graph Neural Network can be used to predict how well kids will do in school. To help students do better, it is suggested that a systematic literature review be done on how to predict student success by using data processing methods.

**Chapter 12:** This chapter shows how artificial intelligence and inspired algorithms can be used to find fake news by using graph neural networks.

**Chapter 13:** This chapter is an in-depth look at face recognition using feature extraction and the fusion face method. The main goal of this chapter is to use image fusion to solve the problem of face recognition. It also gives a thorough look at the different image fusion methods for face recognition.

The book is written in a clear and concise manner, making it easy to understand for anyone with a basic knowledge of machine learning and graph theory. Each chapter includes numerous examples and illustrations to help readers understand the concepts and techniques covered in the book.

The targeted audience for the book includes professionals who are researchers (faculty members and graduate students), and those who would like to learn about this field. This book is expected to have the following specific salient features:

- To serve as a single comprehensive source of information and as reference material on Graph Neural Network.
- To help those who are interested in exploring and implementing the GNN and related technologies
- To deal with an important and timely topic of emerging Graph Neural Network
- of today, tomorrow, and beyond.
- To present accurate, up-to-date information on a broad range of topics related to Graph Neural Network

This book *Concepts and Techniques of Graph Neural Networks* has had a significant impact on the field of graph neural networks (GNNs) and has made valuable contributions to the subject matter.

Firstly, the book provides a comprehensive overview of GNNs, covering the key concepts, techniques, and applications of this emerging field. It explains how GNNs can be used to analyze and model complex graph data such as social networks, biological networks, and recommendation systems. This provides an overview of the basic concepts and terminology used in graph theory, including graphs, nodes, edges, and adjacency matrices. This part of the book is designed to introduce readers to the fundamental concepts of graph theory, which form the basis for understanding GNNs.

Secondly, the book introduces several new techniques for GNNs, such as graph attention networks (GATs), graph convolutional networks (GCNs), and graph autoencoders (GAEs). These techniques have been widely adopted and have significantly improved the performance of GNNs in various applications.

Thirdly, the book highlights the challenges and open problems in GNNs, such as scalability, interpretability, and adversarial attacks, which have stimulated further research in the field.

Overall, the book has had a significant impact on the field of GNNs, providing a solid foundation for researchers and practitioners to develop new models and applications. Its contributions to the subject matter have advanced the understanding of GNNs and paved the way for future research in this exciting and rapidly evolving field.

The authors have carefully designed this book to be accessible to readers with a basic understanding of Graph theory and machine learning. However, readers who are new to these topics may find it helpful to review some of the relevant material before beginning the book. Additionally, readers who are already familiar with GNNs may find the book useful as a reference for specific topics.

Throughout the book, the authors have focused on providing clear explanations of the concepts and techniques presented. They have also included numerous examples and code snippets to help readers understand the material. However, the authors acknowledge that the field of GNNs is rapidly evolving, and some of the material presented in this book may become outdated over time.

The authors would like to thank the many researchers and practitioners who have contributed to the development of GNNs over the years. They would also like to thank the reviewers who provided valuable feedback during the preparation of this book.

## ***Preface***

In conclusion, we hope that this book will provide readers with a clear and comprehensive introduction to the concepts and techniques of Graph Neural Networks. We believe that GNNs will continue to be an important area of research in the years to come, and we hope that this book will inspire further exploration and innovation in the field.

In writing this book, we hope to provide a valuable resource for anyone interested in GNNs, whether they are researchers, practitioners, or students. We believe that this book will serve as a useful reference for years to come and will contribute to the continued growth of the field of GNNs. We hope that readers will find the book informative and enjoyable, and we welcome feedback and suggestions for future editions.

*Vinod Kumar*

*Koneru Lakshmaiah Education Foundation (Deemed), India*

*Dharmendra Singh Rajput*

*VIT University, India*

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We would like to express our heartfelt gratitude to everyone who has contributed to the creation of this book.

First and foremost, we would like to thank the researchers and practitioners in the field of graph neural networks (GNNs) whose groundbreaking work has inspired us to write this book. Their tireless efforts in advancing the understanding and application of GNNs have paved the way for new discoveries and innovations in this exciting field.

We also extend our gratitude to the reviewers who provided valuable feedback and constructive criticism that helped us to refine and improve the content of this book. Their insightful comments and suggestions have helped to ensure the accuracy, clarity, and relevance of our work.

We would like to thank our colleagues and collaborators who have provided support, advice, and encouragement throughout the development of this book. Their contributions have been invaluable, and we are grateful for their expertise and guidance.

We are deeply indebted to our families and loved ones who have supported us through the ups and downs of the writing process. Their patience, understanding, and unwavering support have been essential to our success.

Finally, we would like to express our gratitude to the team at publisher end, who have worked tirelessly to bring this book to fruition. Their professionalism, expertise, and dedication have been essential to the success of this project.

Thank you all for your contributions to this book and to the field of graph neural networks. We hope that this book will inspire new ideas and advancements in this exciting and rapidly evolving field.



# Chapter 1

## Fundamentals of Graph for Graph Neural Network

**Vinod Kumar**

 <https://orcid.org/0000-0002-3495-2320>

*Koneru Lakshmaiah Education Foundation, Guntur, India*

**Himanshu Prajapati**

*United Institute of Technology (UIT), Prayagraj, India*

**Sasikala Ponnusamy**

*Makhanlal Chaturvedi National University of Journalism and Communication, India*

### ABSTRACT

*The vertices, which are also known as nodes or points, and the edges, which are responsible for connecting the vertices to one another, are the two primary components that make up a graph. Graph theory is the mathematical study of graphs, which are structures that are used to depict relations between items by making use of a pairwise relationship between them. Graphs can be thought of as a visual representation of a mathematical equation. The principles of graph theory will be covered in this chapter.*

### INTRODUCTION

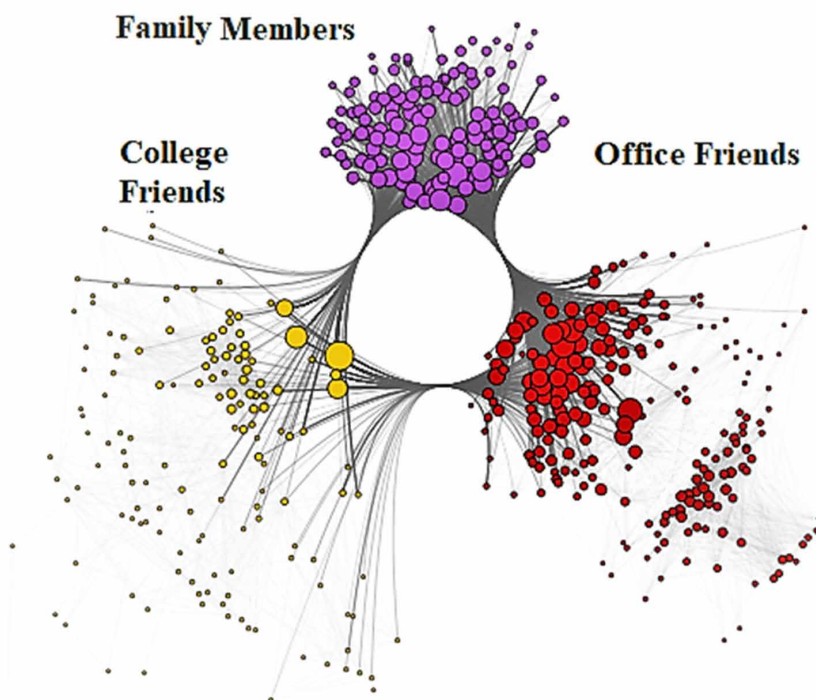
A graph is a useful tool for visually representing any type of physical scenario with distinct objects and some sort of connection between those objects. Many problems are easy to state and have natural visual representations. Nowadays, there are a wide range of applications of graph theory in real life. such as designing a family tree, a computer network, the flow of computation, data organization, finding the shortest path on a road, designing circuit connections, parsing a language tree, constructing the molecular structure, social networking, representing molecular structures, and many more. The publication written by Euler in 1736, in which he solved the Konigsberg bridge problem, is considered to be the birth year of graph theory (Deo, 2017). The importance of graphs in graph neural networks (GNNs) cannot be overstated. Graphs are the fundamental data structure that GNNs operate on and enable the representa-

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tion of complex relationships and dependencies between entities. In many real-world applications such as social networks, recommender systems, drug discovery, and traffic flow prediction, the data can be naturally represented as graphs. Graphs provide a flexible and powerful framework for modeling such data and capturing the dependencies between entities (Ray, 2013). GNNs leverage the graph structure to learn meaningful representations of nodes and edges by propagating information across the graph. They use techniques such as message passing and graph convolutions to iteratively aggregate information from neighboring nodes and update node representations. Moreover, graphs provide a natural way to model inductive transfer learning, where the learned representations from one graph can be transferred to another graph with a similar structure. This is particularly useful in domains such as drug discovery and recommender systems, where the graph structure is similar across different datasets. The importance of graphs in GNNs lies in their ability to model complex relationships and dependencies between entities, their flexibility in representing different types of data, and their usefulness for inductive transfer learning (Zhou et al., 2020).

A graph may be used to represent a variety of different objects, including social media networks and molecules. Consider the nodes to be the users, and the edges to be the connections. Figure 1 is an example of what a graph for social media may look like:

*Figure 1. A sample graph for social media*



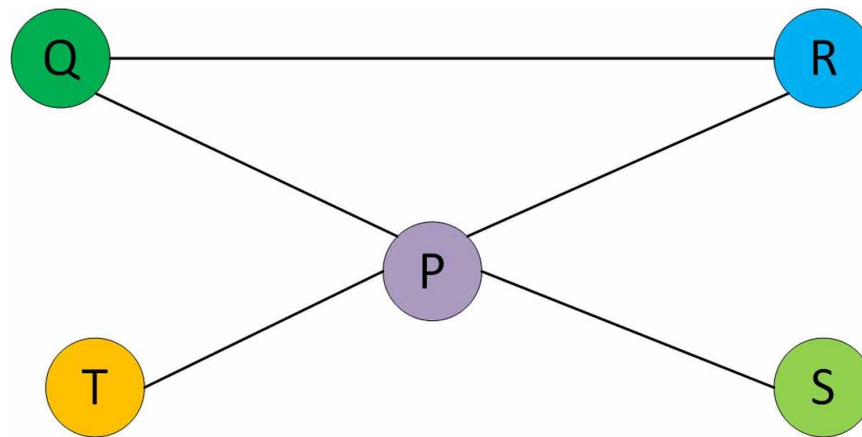
## BACKGROUND OF GRAPH

A network can be represented mathematically as a graph, (Deo, 2017) and a graph's purpose is to depict the relationship that exists between lines and points. The components of a graph are points and the lines that link those points. It does not make a difference how long the lines are or where the points are located. A “node” is the name given to each individual component of a graph. The graph may be seen in Figure 2 and contains 5 vertices and 5 edges (Ray, 2013).

**Def:** A non-empty collection of vertices or nodes  $V$  and a set of edges  $E$  are required for the definition of a graph, which is written as  $G = (V, E)$ . The letter  $G$  identifies the graph here.  $E(G)$  or just  $E$  signifies the edge, whereas  $V(G)$  or simply  $V$  denotes the vertices of a polygon (Deo, N. (2017).

Let us take, a graph  $G = (V, E)$  where  $V = \{P, Q, R, S, T\}$  and  $E = \{\{P, Q\}, \{Q, R\}, \{P, R\}, \{P, S\}, \{P, T\}\}$ .

*Figure 2. Graph with and five edges five vertices*



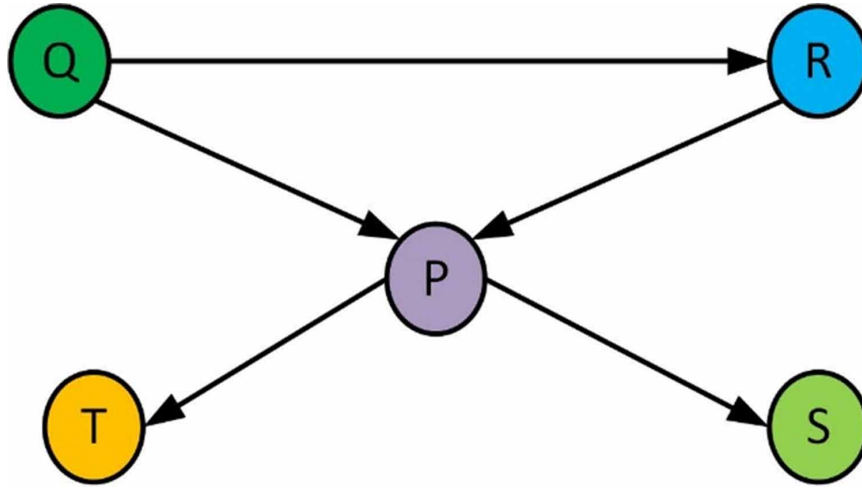
### Directed Graph

A directed graph (digraph) (Trudeau, 2013) is a graph that involves the collection of vertices connected by edges, where each edge also has a direction (Deo, 2017). Figure 3 demonstrates the directed graph with five edges and five vertices.

### Undirected Graph

An undirected graph is arrangement of vertices  $V = \{P, Q, R, S, T\}$  connected by edges  $E = \{\{P, Q\}, \{Q, R\}, \{P, R\}, \{P, S\}, \{P, T\}\}$ , where each edge has no direction. Figure 1 demonstrates an example of undirected graph with five vertices and five edges (Deo, 2017).

Figure 3. Directed graph with five vertices and five edges



## Simple Graph

An undirected graph without parallel edges or self-loops is called as simple graph. Figure 1 is an illustration of simple graph with five vertices and five edges (Deo, 2017).

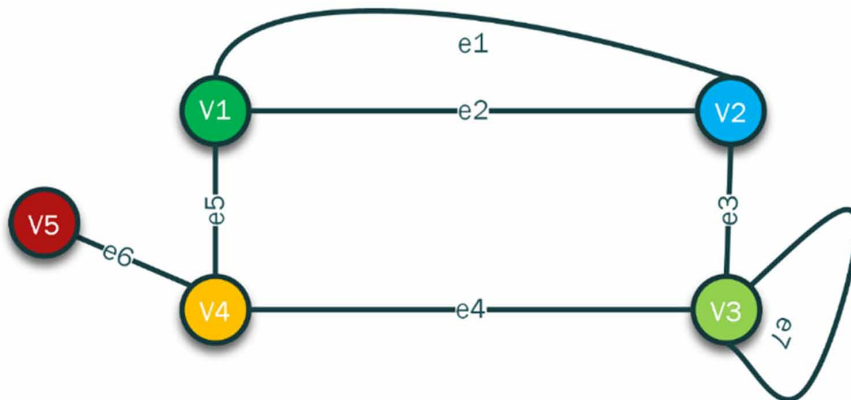
## Incidence and Degree

The number of branches coming on a node  $v_i$  is named as the degree,  $d(v_i)$  of vertex  $v_i$ .

Figure 4 consists of five vertices  $\{v_1, v_2, v_3, v_4, v_5\}$  and seven edges  $\{e_1, e_2, e_3, e_4, e_5, e_6, e_7\}$

Here,  $d(v_1) \rightarrow 3$ ,  $d(v_2) \rightarrow 3$ ,  $d(v_3) \rightarrow 4$ ,  $d(v_4) \rightarrow 3$ ,  $d(v_5) \rightarrow 1$

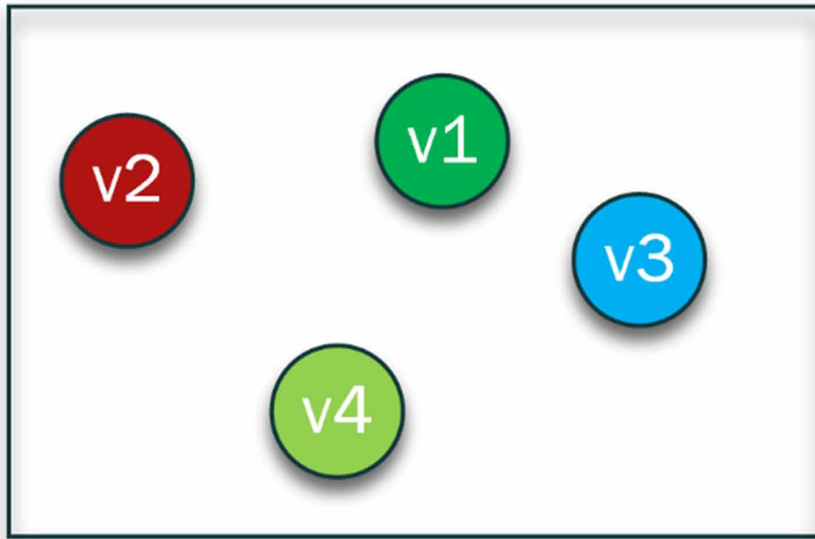
Figure 4. A graph having five vertices and seven edges



## **Null Graph**

Let's say  $G = (V, E)$ . In this case, there is a chance that the edge set  $E$  is empty. A “null graph” is a graph that doesn't have any edges. In other words, every point in a graph with no edges is an isolated point. Figure 5 shows a graph with no edges and four points (Deo, 2017).

*Figure 5. Null graph with four vertices*



## **Multigraph**

A graph that does not follow any particular direction and does not contain any loops or multiple edges (Trudeau, 2013). Whereas a graph with multiple edges between the same set of vertices and has loops formed. It is called Multigraph (Deo, 2017). In Figure 6. Vertices  $v2$  and  $v3$  have multiple edges. Hence Figure 5 is an example of multigraph.

## **Finite and Infinite Graph**

A graph is said to be finite (Deo, 2017) if it has a certain limit on the number of vertices and edges that it contains. On the other hand, a graph that is said to have an unlimited number of vertices and edges is said to be an infinite graph (Ray, 2013). An illustration of an infinite graph is shown in Figure 7.

Figure 6. Multigraph

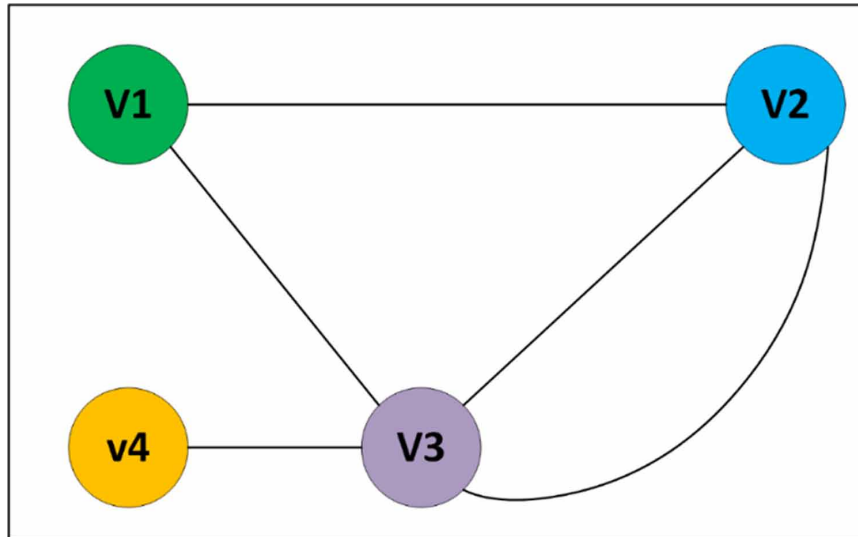
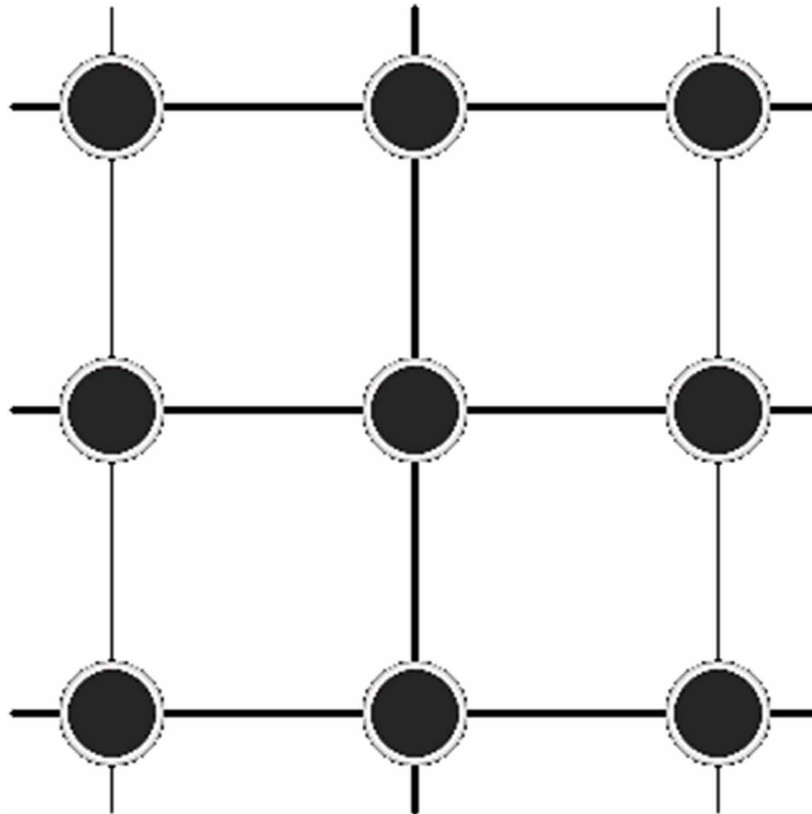


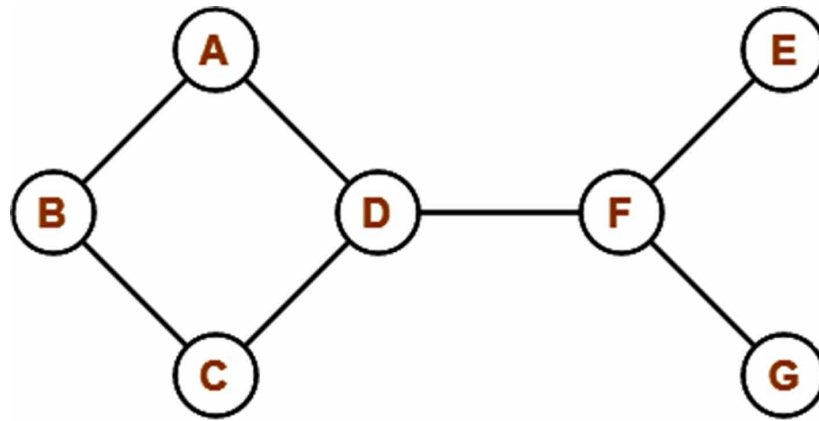
Figure 7. Infinite graph



## Connected Graph

The term “connected graph” refers to a type of graph in which it is possible to travel from any one vertex to any other vertex (Ray, 2013). In a connected graph, there is always at least one path that may be taken from one pair of vertices to the next (Deo, 2017). Figure 8 shows connected graph with seven vertices and seven edges.

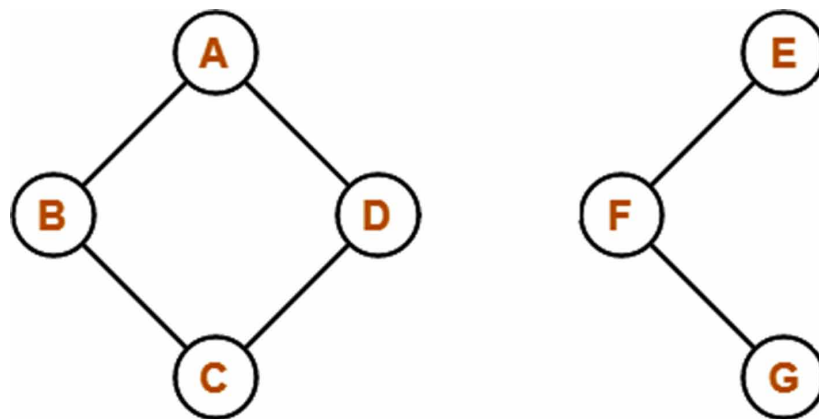
*Figure 8. Connected graph with seven vertices and seven edges*



## Disconnected Graph

A type of graph in which any two adjacent vertices or nodes are separated by a path (Deo, 2017). Figure 9 an illustration of a graph that is detached from its source.

*Figure 9. Disconnected graph*



## Regular Graph

When all of the vertices in a graph have the same degree, we say that the graph is regular (Deo, 2017). Each vertex of a regular graph  $G$  of degree  $d$  has the same value for its degree, which is  $d$ .

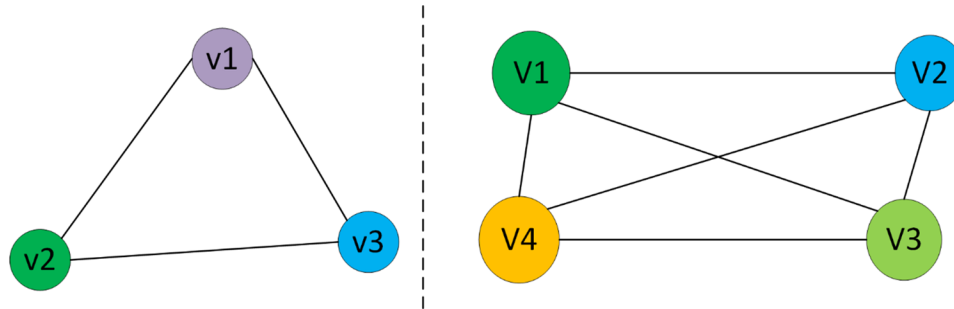
## Complete Graph

When every pair of vertices in a structure is connected by exactly one edge, we refer to the graph as a complete graph.  $K_n$  is the notation used to refer to a complete graph (Ray, 2013; Trudeau, 2013). that has  $n$  vertices.

- The number of edges in a complete graph with  $n$  vertices is precisely equal to  ${}^nC_2$ .
- The value  $K_n$  is the representation of a complete network with  $n$  vertices.

Figure 10 depicts two complete graphs, one with three vertices and the other with four.

Figure 10. Complete graph



## Cycle Graph

The term “cycle graph” refers to a graph that only contains one cycle over its entirety. The term “cycle graph” refers to a basic graph that contains “ $n$ ” vertices ( $n \geq 3$ ) and “ $n$ ” edges, all of which come together to form a cycle of length “ $n$ .” In a graph depicting a cycle, each of the vertices has a degree of 2.  $C_n$  is the abbreviation for the cycle graph that has  $n$  vertices (Deo, 2017).

Every vertex in the  $C_n$  graph has a degree of 2, and the number of vertices in  $C_n$  is equal to the number of edges.

Figure 11 shows four different examples of cycle graphs using the components  $C_3$ ,  $C_4$ ,  $C_5$ , and  $C_6$ .

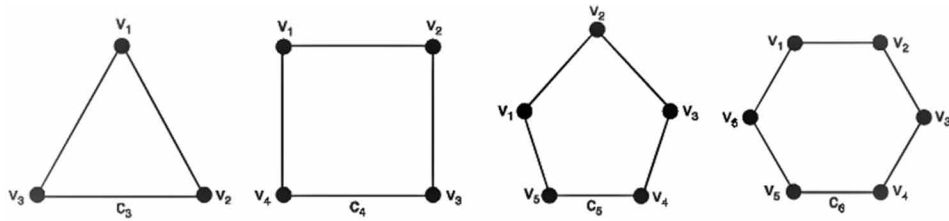
In a directed variant of a cycle graph known as a directed cycle graph, each of the edges in the graph is orientated in the same direction as the other edges.

**In Degree:** The number of edges coming into a vertex in a directed graph (Ray, 2013; Trudeau, 2013).

**Out Degree:** The number of edges going out from a vertex in a directed graph (Ray, 2013; Trudeau, 2013).



*Figure 11. Cycle graphs with  $C_3$ ,  $C_4$ ,  $C_5$ ,  $C_6$*

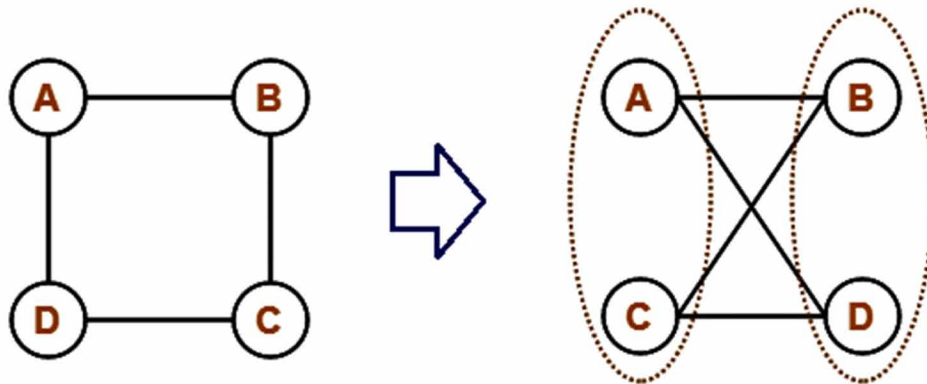


## **Bipartite Graph**

Bipartite graphs are an extremely intriguing example of geometrical design (Arunkumar & Komala, 2015). This has a wide range of applications, including cancer detection, advertising and e-commerce ranking systems, forecasting preferences (for things like movies or foods), and solving matching difficulties (stable marriage problem). The Bipartite Graph is depicted with four vertices and eight verities, respectively, in Figures 12 and 13. A graph with two distinct halves is called a bipartite graph (Deo, 2017).

A graph is said to be bipartite if its vertices are able to be partitioned into two distinct sets named X and Y. The vertices of set X can only connect with the vertices of set Y in order to form a connection. None of the vertices that belong to the same set are connected to one another in any way (Deo, 2017).

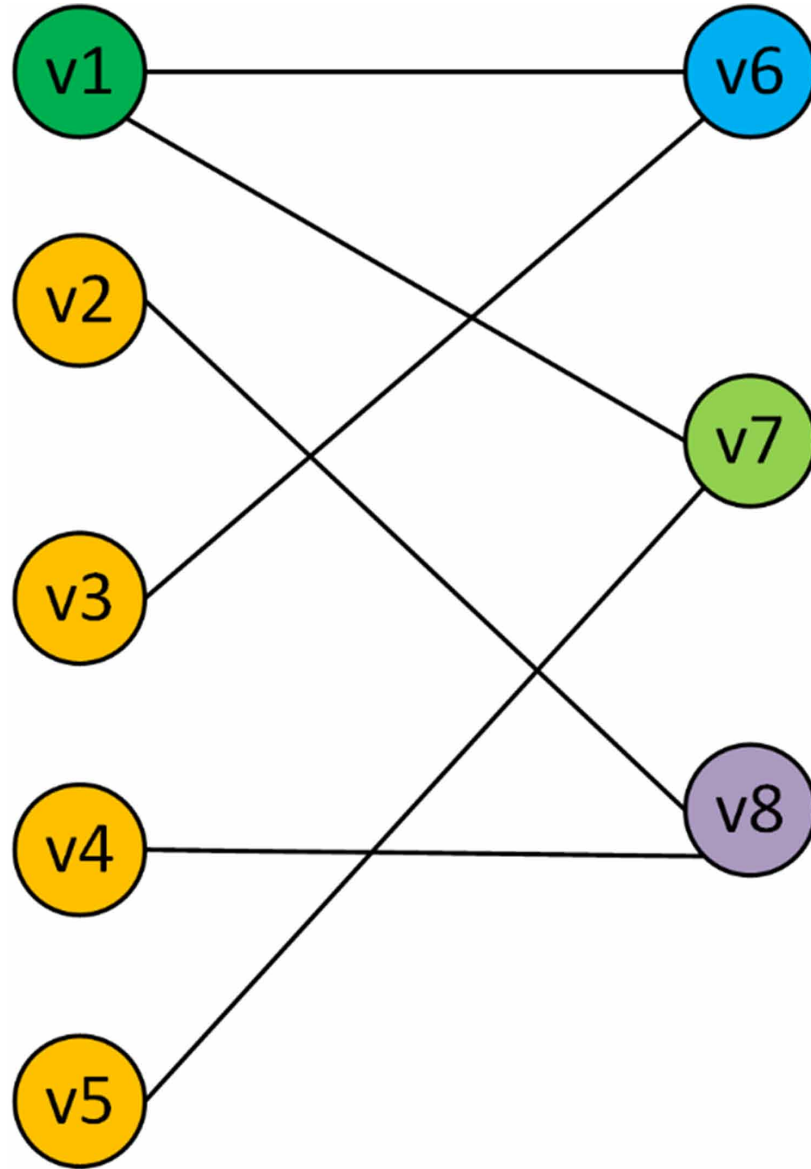
*Figure 12. Bipartite graph with four vertices*



## **Representation of Graphs**

The process of storing a graph within the memory of a computer is referred to as a graph representation. two main ways to represent a graph are discussed here.

Figure 13. Bipartite graph with eight vertices



### Adjacency Matrix

The  $n$  by  $n$  matrix  $A$ , which is indexed by  $V$ , is the adjacency matrix (Ray, 2013; Trudeau, 2013) for the equation  $G = (V, E)$ , and the entry for  $(v_i, v_j)$  is defined as:

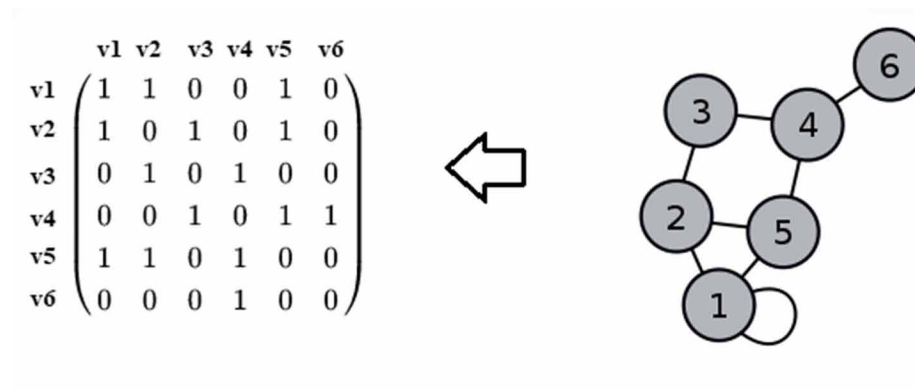
$$\{ A_{v_i, v_j} = 1 \text{ if } v_i, v_j \in E, \text{ Otherwise } 0 \}$$

The adjacency matrix, also known as the connection matrix, is a square matrix with rows and columns that is used to represent a basic labeled finite graph, with 0 or 1 in the position  $(v_i, v_j)$  based on whether  $v_i$  and  $v_j$  are adjacent or not. Vertex matrix is another name for adjacency matrix. If the simple graph contains no self-loops, then the diagonal of the vertex matrix should contain 0.

Undirected graphs are symmetrical. The connection matrix is a square array with rows representing graph out-nodes and columns representing graph in-nodes. Entry 1 represents a graph edge between two nodes. The  $i^{\text{th}}$  row and  $j^{\text{th}}$  column has the same value. Figure 14 represents the adjacency matrix.

*Figure 14. Adjacency matrix*

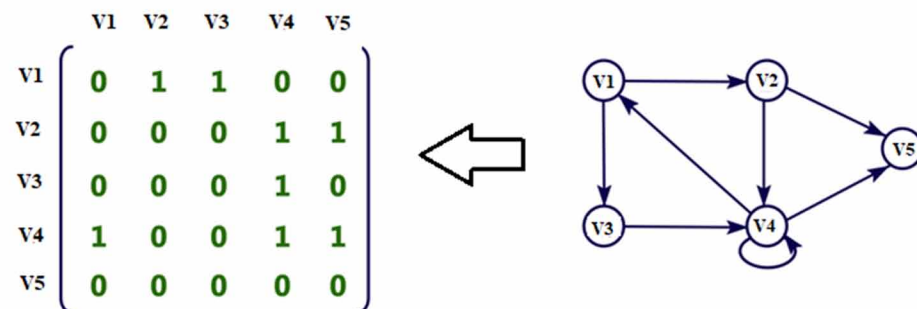
**Note:** If the graph is weighted, we can save the edge weight instead of 1s and 0s.



## Adjacency Matrix of a Directed Graph

Edges in a directed graph denote a particular route that can be taken to get from one vertex to another vertex. If there is a path that goes from one vertex A to another vertex B, then node A is considered to be the starting node, and node B is considered to be the finishing node. Figure 15. displays the adjacency matrix of a directed graph (Deo, 2017).

*Figure 15. Adjacency matrix of a directed graph*

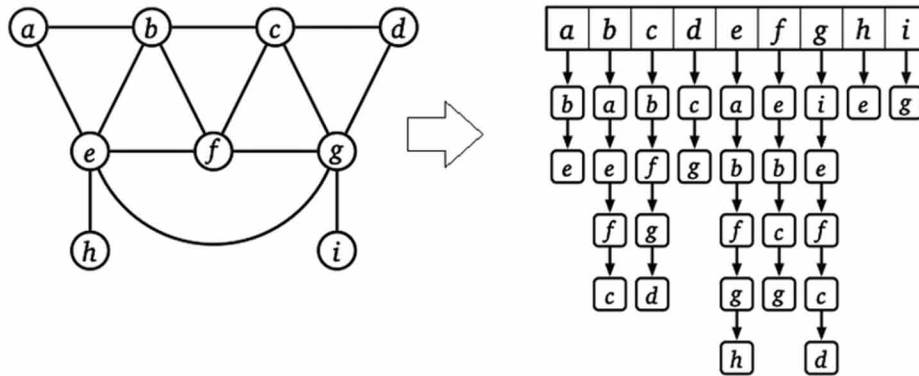


## Adjacency List

Adjacency lists (Ray, 2013 & Trudeau, 2013). express graphs as linked lists. Most graphs use adjacency lists. Its unusual shape makes it easy to distinguish which vertices are adjacent. Linked lists let graph vertices reference their neighbours (Deo, 2017).

For each node in the graph, an adjacency list is kept that stores the node value and a pointer to the next neighboring node to the respective node. If all adjacent nodes have been traversed, then the pointer field of the end node in the list should be set to NULL. Figure 16 shows the adjacency list.

Figure 16. Adjacency list



## Heterogeneous Graph

A heterogeneous graph is a type of graph where nodes and edges can have different types and attributes. In other words, each node and edge in the graph can belong to a different category or class, and can have different properties or characteristics. Heterogeneous graphs are used to represent complex systems that involve multiple types of objects and relationships, such as social networks, recommendation systems, and knowledge graphs.

In a heterogeneous graph, nodes and edges are usually labeled with types or attributes that describe their properties. For example, in a social network, nodes could be labeled with attributes such as user age, gender, occupation, and interests, while edges could be labeled with attributes such as friendship, follow, or like. In a recommendation system, nodes could be labeled with attributes such as user preferences, item features, and ratings, while edges could be labeled with attributes such as purchase, view, or click.

Heterogeneous graphs have several advantages over homogeneous graphs, where all nodes and edges have the same type. First, they can represent more complex relationships between objects, such as hierarchical relationships, multi-relational networks, and contextual dependencies. Second, they can capture richer information about objects and their properties, which can be used to improve machine learning models and data analysis. Finally, they can enable more flexible querying and retrieval of information from the graph, since users can specify queries that involve different types of nodes and edges.

Heterogeneous graphs have several applications in machine learning and data mining, including recommendation systems, entity matching, link prediction, and graph embedding. Heterogeneous graph-based algorithms have been shown to outperform traditional homogeneous graph-based algorithms in many tasks, especially when dealing with complex and diverse data.

## Graph Embedding

Graph Embedding is a technique used in Graph Neural Networks (GNNs) to represent each node and the overall graph as a low-dimensional vector or embedding (Velickovic et al., 2018). These embeddings capture important structural and semantic information about the nodes and edges in the graph, which can be used for a wide range of downstream tasks, such as node classification, link prediction, and graph clustering.

There are different ways to generate graph embeddings in GNNs, but the most common approach is through message passing. In this approach, each node sends and receives messages to and from its neighbors, and aggregates this information to update its own representation or embedding. The messages typically consist of information about the neighboring nodes and edges, such as their features or weights, and the aggregation functions can be simple ones like sum or max, or more complex ones like attention or graph convolution (Wu et al., 2020, 2022).

As the message passing process continues over multiple iterations or layers, the embeddings of the nodes and the graph become increasingly refined and informative, allowing GNNs to capture complex patterns and dependencies in the graph structure and features. The final node and graph embeddings can then be used as inputs to downstream tasks or as features for visualization and analysis.

Let's take a Graph  $G = (V, A, X)$  such that:

$V$ - vertex set,  $A$ -is the adjacency matrix,  $X \in \mathbb{R}^{m \times |V|}$  is the node feature matrix

An explanation of how a single node compiles the messages received from its immediate surroundings. The model collects messages from  $A$ 's local graph neighbours (i.e.,  $B, C$ , and  $D$ ), and the messages arriving from these neighbours are based on information collected from their respective neighbourhoods. This process continues until all messages have been collected.

The message-passing paradigm is depicted here in its two-layer variant that is shown by Figure 17. It should be noted that the computation graph of the GNN takes the shape of a tree when the neighbourhood surrounding the target node is unfolded.

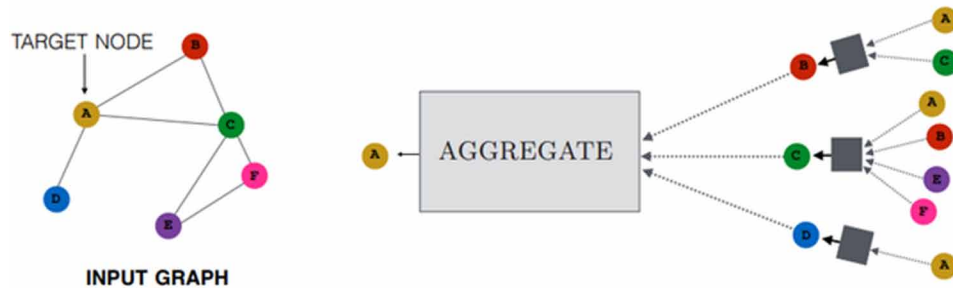


Figure 17. Computational graph and generalized convolution

Figure 18. Computational graph on  $G$  with two layers

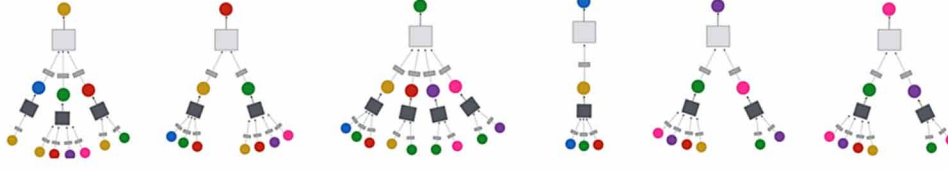
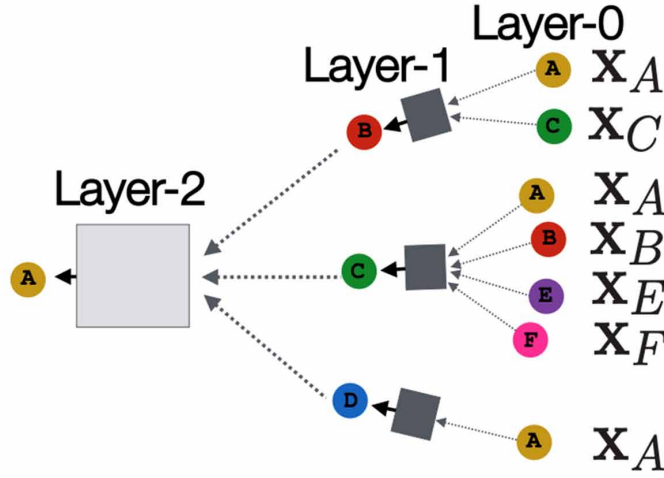


Figure 19. computational graph for node



## Dynamic Graph

A dynamic graph is a graph that changes over time. In the context of graph neural networks (GNNs), a dynamic graph refers to a graph that is not static and can evolve based on various factors, such as new node or edge additions, node or edge deletions, and changes in node or edge attributes (Kumar & Thakur, 2017).

Handling dynamic graphs is important for many real-world applications, such as social network analysis, recommendation systems, and traffic prediction. To handle dynamic graphs, researchers have proposed various approaches for GNNs, including (Scarselli et al., 2008).

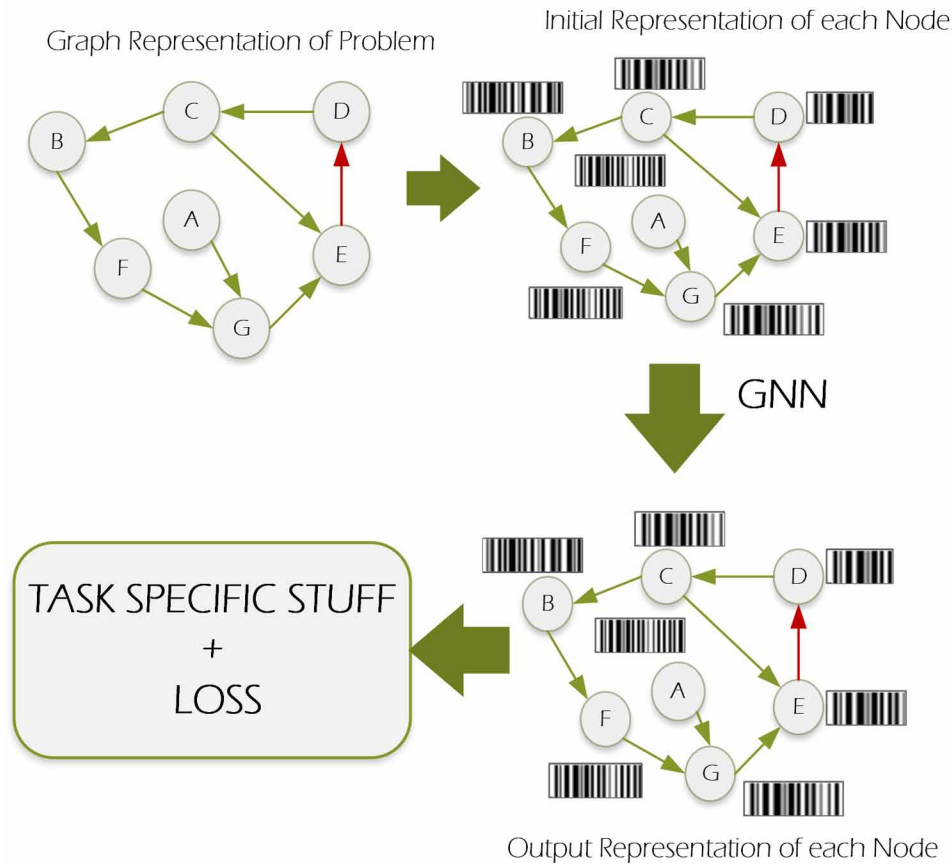
1. **Temporal GNNs:** Temporal GNNs model the evolution of the dynamic graph over time by incorporating temporal information into the GNN architecture. This can be done by adding a time dimension to the input features of the GNN, or by using recurrent neural networks to capture temporal dependencies.
2. **Graph Streaming:** Graph streaming methods process the dynamic graph as a stream of edges or nodes, rather than as a whole graph. This allows the GNN to adapt to changes in the graph over time.

3. **Graph Editing:** Graph editing methods update the graph representation based on changes to the graph structure or attributes. This can be done by adding or removing nodes and edges, or by updating the attributes of existing nodes and edges.
4. **Graph Attention:** Graph attention methods dynamically update the attention weights of the GNN based on changes to the graph structure or attributes. This allows the GNN to focus on important nodes and edges in the dynamic graph.

Overall, handling dynamic graphs is an active area of research in GNNs, and there are many exciting developments in this field.

Graph theory provides a powerful framework for understanding the structure and properties of graphs, and is essential to the development and analysis of GNNs. Information given in Table 1 are just a few examples of the ways in which Graph Theory is used in Graph Neural Networks. Depending on the specific application and task at hand, other concepts and techniques from Graph Theory may also be relevant.

*Figure 20. Graph representation of problem in GNN*



*Table 1. Summary table of some of the ways in which graph theory is used in graph neural networks*

SN	Graph Theory Concept	Description	Applications in GNN
1	Graph structure	The arrangement of nodes and edges in a graph	Used to represent input data and compute node/edge embeddings
2	Node degree	The number of edges connected to a node	Used to compute node embeddings and graph properties
3	Adjacency matrix	A matrix representation of the edges in a graph	Used to define the graph structure and compute node/edge embeddings
4	Laplacian matrix	A matrix derived from the adjacency matrix that captures graph connectivity and properties	Used to compute spectral node embeddings and graph properties
5	Graph connectivity	The extent to which nodes in a graph are connected to each other	Used to compute node and graph-level properties, such as clustering coefficients and centrality measures
6	Random walks	A path through a graph that is determined by a series of random choices	Used to generate node sequences and compute node embeddings
7	Graph clustering	The grouping of nodes in a graph based on their similarity or connectivity	Used to partition graphs and compute node/cluster embeddings
8	Community detection	The identification of subgroups of nodes that are more densely connected to each other than to the rest of the graph	Used to partition graphs and compute node/community embeddings
9	Graph generation	The creation of new graphs that exhibit certain properties or characteristics	Used to generate synthetic data and test GNN performance on novel graphs
10	Graph isomorphism	A concept of equivalence between different representations of the same graph	Graph isomorphism is used to ensure that the same graph is represented consistently across different layers of a GNN
11	Shortest paths	Shortest paths, which measure the minimum number of edges needed to traverse from one node to another.	Shortest paths, can be used in GNNs to capture the proximity of nodes in the graph.

## WHY IS IT HARD TO ANALYSE A GRAPH IN GNN?

Analyzing a graph in a Graph Neural Network (GNN) (Scarselli et al., 2008) can be challenging for several reasons:

1. **Complexity:** GNNs can handle very complex graphs, which can make it challenging to identify patterns and relationships. The number of nodes and edges can be very high, and the structure of the graph can be irregular, making it difficult to analyze.
2. **Interpretation:** GNNs use a distributed representation of the graph that can be difficult to interpret. Each node in the graph is represented as a high-dimensional vector, and the relationship between nodes is encoded in the connections between these vectors. Interpreting these vectors and the relationships between them requires a deep understanding of the underlying algorithms and domain-specific knowledge.
3. **Training:** GNNs require large amounts of training data, which can be difficult to obtain for some applications. In addition, training GNNs can be computationally expensive and requires expertise in deep learning and optimization.



4. **Overfitting:** GNNs can be prone to overfitting, where the model memorizes the training data instead of learning general patterns. Overfitting can occur when the graph is too complex or when the model is too powerful, and can lead to poor performance on new data.
5. **Performance:** GNNs can be slow and computationally expensive, particularly for very large graphs. Optimizing the performance of GNNs requires careful tuning of hyperparameters and efficient use of hardware resources.

Of course, analyzing a graph in a GNN can be a challenging task that requires a combination of technical skills, domain knowledge, and analytical thinking. However, GNNs can be a powerful tool for understanding complex data sets and identifying meaningful patterns and relationships, particularly in applications such as social networks, recommendation systems, and drug discovery.

## **CONCLUSION**

The Graph Neural Networks (GNNs) are a type of neural network that operate on graph data structures. Therefore, understanding the fundamentals of graph theory is essential to grasp the basic concepts of GNNs. Graphs consist of nodes (also known as vertices) and edges (also known as connections), and can represent a wide variety of data, including social networks, protein interactions, and road networks. This chapter contains discussion of basic Important key terminologies related to graphs such as graph and its various types, nodes, edges, degree of a graph, adjacency matrix, representation of graphs, graph embedding, etc.

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## KEY TERMS AND DEFINITIONS

**Dynamic Graph:** A dynamic graph is a graph that changes over time.

**Graph:** In mathematics and computer science, a graph is a collection of points, called vertices or nodes, connected by lines or arcs, called edges. Graphs are often used to model relationships between objects, with the nodes representing the objects and the edges representing the relationships between them.

**Graph Embedding:** Graph Embedding is a technique used in Graph Neural Networks (GNNs) to represent each node and the overall graph as a low-dimensional vector or embedding.

**Graph Neural Networks (GNNs):** GNNs are a type of neural network that is designed to operate on graph-structured data, which is a type of data that is naturally represented as a set of nodes and edges. In a GNN, each node in a graph is associated with a vector representation, which is updated based on the node's own features as well as the features of its neighbors in the graph. The goal of a GNN is typically to perform some kind of prediction or classification task on the graph-structured data, such as predicting the category of a node or predicting the presence of certain types of edges in the graph.

**Simple Graph:** An undirected graph without parallel edges or self-loops is called as simple graph.

## Chapter 2

# Graph Neural Network and Its Applications

**Sougatamoy Biswas**

*National Institute of Technology, Rourkela, India*

### ABSTRACT

*Graph neural network (GNN) is an emerging field in deep learning. Graphs have more expressive power than any other data structure. Graph neural network is one of the application areas of deep learning, and it has applications in different domains where traditional convolutional neural networks can't give the desired result. Graphs are basically connections of nodes through the edges. In the area of recommendation systems, image processing and fraud detection are some of the few application areas of graph neural networks. As graphs are moveable and mobile in nature, they are more flexible to apply in these domains. GNN deals with these types of problems more effectively than a convolution neural network. To apply GNN to a specific problem domain, data needs to be converted into a graphical format, and then neural network operations can be executed. The main feature of GNN is to inherit information from its neighborhood. This is called graph embedding. This chapter describes basic GNN architecture, GNN advantage over CNN, and its application in different domains.*

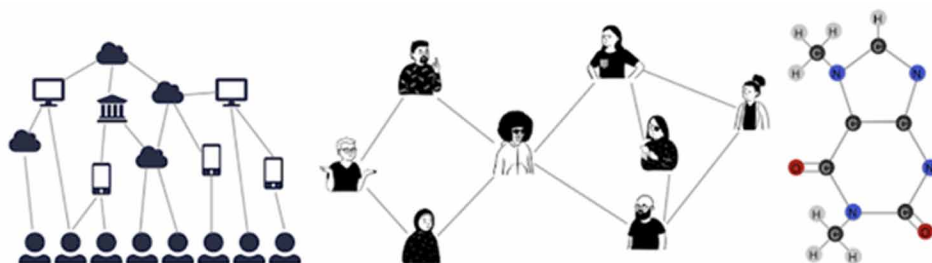
### INTRODUCTION

Graph structure data can be represented in various application fields like natural language processing, image processing, and software engineering. Graphical format data can be processed by Graph Neural Networks (GNNs). Graphs are a fundamental way to represent data that have complex relationships between elements. They are widely used in various domains, such as social network analysis, molecular chemistry, computer vision, and natural language processing. Recently, GNNs have attracted a lot of interest in both the academic and business communities for applying graphs. Classifying nodes, link prediction, and graph clustering are just some of the many downstream tasks and GNN might extract semantic information from these networks. Unlike traditional neural networks that operate on regular grids, such as images and sequences, GNNs operate on irregular graph structures, presenting unique challenges in modeling the relationships between the nodes.

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The development of GNNs has been driven by advances in deep learning and graph theory. The first GNN was proposed by (Scarselli et al., 2009), which used a recurrent neural network to propagate information between nodes in a graph. The range of possible uses for GNNs is enormous. Image categorization, object recognition, and semantic segmentation are just some of the computer vision applications that GNNs have been used. For many years, GNNs have been utilized for phrase categorization, entity identification, and relation extraction in the field of natural language processing. GNNs have been implemented for a variety of tasks in social network analysis, including link prediction, node categorization, and community discovery. In the field of molecular chemistry, GNNs have been used for tasks such as drug discovery and molecular property prediction. Single nodes and sequences are the most basic graph structures. Graph data structures are mobile in nature and that's the reason the convolution neural networks cannot process this complicated type of mobile data structure (Scarselli et al., 2009) as it works mainly on static data structure. That is where GNN came into the picture. Nodes and edges make up the data structure known as a graph. Each node in the graph is an entity and the relationship between the entities are defined as edges; these relationships may be established using any suitable similarity metric.

Figure 1. Graph models between different types of data



Graphs have great expressive power and it's the reason GNN (Huang et al., 2019) can be used in many domains such as molecule interaction, natural science, machine learning, and many more research areas. Graph structure can be facile with basic nodes and edge connection, or it may be perplexing in nature like trees, acyclic graphs, or cyclic graphs. In machine learning, problem analysis through graphs acts as a unique non-Euclidian data structure (Shchur et al., 2018) that mainly focuses on node classification, clustering, and connection prediction. Classification is one of the prominent areas where GNN is used. In the classification problem (Fu et al., 2020) each node has a label and without using ground-truth labels the nodes need to be predicted.

## BACKGROUND

Because of the ability to process input that is organized as a graph the Graph Neural Network (GNN) has gained lots of popularity in the recent times. In several applications, such as NLP, computer vision, drug discovery and graphical network analysis, GNNs have shown to be effective. The first-time graph neural network was proposed back in 2005 (Scarselli et. al., 2005) to apply the concept of graph data and

from then it has gained its popularity. Throughout time all this research has enhanced the application of GNN in different areas. Some of the most popular research works are mentioned here.

This literature review aims to introduce readers to GNNs and their numerous potential applications. We will discuss the different GNN architectures and their characteristics, as well as their applications in computer vision, natural language processing, social network analysis, and molecular chemistry. We'll talk about some of the obstacles and potential futures in GNN study as well.

Wang et al. (2017) enhanced its application with recurrent networks and other optimization technique. Graph neural networks collects neighborhood information from the neighboring nodes and combines all information as a feature output. Kipf and Welling (2017) applied Generalized convolution-based propagation rules to semi-supervised learning graph-based data with scalability. Some of the GNN approaches are based on node-labeling framework. CNN in non-Euclidian space explored and traversed by Monet on different graphs and manifolds methods. Bronstein et al. presents a comprehensive overview of geometric in-depth education, including its issues, concerns, approaches, implementations, and suggestions for future.

Focusing on specific application domains, Gilmer et al. (2017) and Wang and Yan (2021) use frameworks of different models and generalize a model without providing review over other GNN models. Wang et al. (2017) explained the graph model review. Battaglia et al. (Battaglia, 2021) generalized other models using graph network framework and explained graph classification models keeping graph network model abstract.

In a study by Wu et al. (2021), GNNs were used for drug discovery tasks such as predicting drug-target interactions and molecular property prediction. For applying GNN into various domains the researchers have implemented Graph Convolution Neural Network (GCN). The GCN can capture the non-linear dependencies among the nodes.

In the domain of computer vision GNN have also been used for classifying and detecting objects. For instance, in a study by Yan et al. (2018), a GNN-based method was proposed for image classification, where the authors used a GNN to learn the relations between the image regions and classify the image. Similarly, in a study by Simonovsky and Komodakis (2017), GNNs were used for 3D object detection, where a volumetric representation of the object was constructed and a GNN was used to learn the object features.

Natural language processing (NLP) is another application where GNNs have showed promise. For instance, in a study by Liu et al. (2019), a GNN-based model was proposed for sentence classification, where a graph was constructed using the words in the sentence, and a GNN was used to learn the sentence features.

GNNs have also been used for social analysis of network, classification of node and predicting link. For example, in a study by Hamilton (2017), a method that is based on GNN has been proposed for predicting the link between the nodes with the information of node embedding.

Finally, GNNs have shown promising results in several different fields, including computer vision, NLP, drug development, and social network research. The use of GNNs in these applications has resulted in significant improvements in performance and opened new possibilities for research. As GNNs continue to evolve, it is expected that they will become an increasingly important tool for solving complex problems in various fields.

## ARCHITECTURE OF GNN

The GNN is merely approached to use the working procedure of node embedding (Schlichtkrull et al., 2018) to learn its neighbor information. For node labelling and edge prediction node embedding can be used. The GCN architecture (Zhang et al., 2019) implements message passing for transferring messages to the neighboring node. These messages are then used to update the node features. The overall process can be represented by the following equations:

Let's say for each node the input feature in the graph is matrix  $X$ , total number of nodes are  $N$  and number of features are  $F$ . The column value represents the node and row value represents the feature dimension. Let  $N$  be the total number of nodes in the graph and  $F$  be the number of features for each node.

$$X \in \mathbb{R}^{(N \times F)} \quad (1)$$

The connection between two nodes in the graph is defined by  $A_{ij}$  where  $A$  is the adjacency matrix. The value of  $A_{ij}=1$  if there is an edge between nodes  $i$  and  $j$ , otherwise 0.

$$A \in \mathbb{R}^{(N \times N)} \quad (2)$$

The weighted sum of the features for each neighbor node is calculated to compute each node updated feature for the adjacency matrix  $A$ :

$$Z = A X \Theta \quad (3)$$

where  $\Theta$  is a weight matrix that transforms the feature dimension.  $Z$  is a matrix of node representations, where the row represents the node and the column represents the feature dimension.

$$Z \in \mathbb{R}^{(N \times F')} \quad (4)$$

where  $F'$  is the output feature dimension, which can be different from the input feature dimension  $F$ . A non-linear activation function ReLU is applied for node representation:

$$H = \sigma(Z) \quad (5)$$

where  $\sigma$  is the activation function.

Finally, we apply another weight matrix  $\Psi$  to obtain the final node features:

$$Y = H \Psi \quad (6)$$

$Y$  is a matrix of updated node features, where each row corresponds to a node and each column corresponds to a feature dimension.

$$Y \in \mathbb{R}^{(N \times C)} \quad (7)$$

where  $C$  is the number of classes for classification tasks. Overall, the GCN architecture can be represented by the following equations:

$$Y = \sigma (A \times \Theta) \Psi \quad (8)$$

For adjacency matrix  $A$ , the input feature matrix is  $X$ ,  $\Theta$  and  $\Psi$  are the weight matrices, the activation function is  $\sigma$ , and  $Y$  is the output feature matrix.

The basic building block of a GNN is the graph convolutional layer. The process of message-passing through the graph is repeated for multiple layers, with each layer receiving as input the output of the previous layer. This allows the GNN to capture increasingly complex representations of the graph structure, as information from distant nodes is gradually incorporated into the node features. The final output of the GNN is a feature vector for each node in the graph.

## GRAPH EMBEDDING

The GNN can operate the way convolution neural network (Kim et al., 2019) is built with the operation of convolution, min, and max pooling operation. The number of layers in GNN is used depends on the network structure, operational complexity of the network and output (Asif et al., 2021).

After converting data into graphical format, it is given as input in GNN which will output a numerical value which will imply the graph node and their relationship (Qiu et al., 2020). The final output is a vector representation from the output layer of GNN and graph embedding will transform the nodes and edges of the graph into a vector space. Embedding is mainly used to convert data from complex to easily understandable format (Shi & Rajkumar, 2020). For example, to convert the words into numerical format graph embedding is used.

### Graph Embedding Process

The process of graph embedding uses the concept of message passing. The nodes of the graph data of GNN with similar features are connected (Jia & Benson, 2020). In case of multiple layers of GNN, they will be repeated. Data will be merged in each layer and forwarded to the next layer.

For example, in social network friend recommendation GNN can be used. First layer will merge the user data and next layer will add it from the friends of friends based on similarity and so on (Guo & Wang, 2021). At the last the output layer will use the embedding to convert it into a vector representation with the node data and its nearby data (Thekumparampil et al., 2018). Representing a graph as a vector or group of vectors in a high-dimensional space is called “embedding” a graph. Graph embedding transforms the information into structured graphical format. One common approach to graph embedding is using a Graph Neural Network (GNN) that maps a graph into a high-dimensional space. The output of the GNN can then be used as the graph embedding.

The input of GNN is an adjacency matrix  $A$  with  $N \times N$  binary matrix and a collection of node characteristics  $X$  is an  $N \times F$  matrix, where  $N$  being the number of nodes in the graph and  $F$  being the number of features per node. The GNN consists of multiple layers, each of which applies a transformation information from its neighboring nodes with node features.

Mathematically, the GNN can be represented as:

$$h^{(l+1)} = f(h^l, A) \quad (9)$$

where  $h^l$  is the features of node and  $l$  represents the corresponding layer,  $h^{(l+1)}$  is the node features at layer  $(l+1)$ , and  $f$  is the graph neural network function with the node features  $h^l$  and the adjacency matrix  $A$  as input.

The final node features at the last layer of the GNN can be used as the graph embedding:

$$Z = h^L \quad (10)$$

where  $Z$  is an  $N \times D$  matrix, with  $D$  being the dimensionality of the embedding space.

The graph embedding  $Z$  is used for different downstream tasks like predicting a link, classifying a node and graph clustering.

The same type of approach is used in convolutional neural networks in extracting output (Xinyi & Chen, 2019). That's the reason convolution operation is preferred for embedding in graph convolutional neural network (GCN).

## ADVANTAGE OF GNN OVER CNN

The primary advantage of GNN is it can be used in those areas where Convolution neural network can't be used (Zhu et al., 2018). Convolution neural network can be used in image processing, object detection etc. CNNs are very useful in tasks like image classification, image recognition, or object detection.

CNN is mainly based on convolution and pooling layers and it can't give desired output with mobile nodes (Gui et al., 2019). It works prominently with fixed network. As per the application CNN applies on graph in a non-Euclidean space whereas GNN applies in a Euclidian space. Therefore, in an image file position mapping of all the pixels are connected in terms of nodes. In an image dataset it doesn't matter with the pixel location in the case of GNN as each pixel is defined as a node in the graph. The adjacent pixels with a relationship will relate to an edge for connection establishment. GNN nodes are always moveable, and a Euclidean space is more unrestricted than non- Euclidean space. In such cases GNN gives more relevant result as output than CNN.

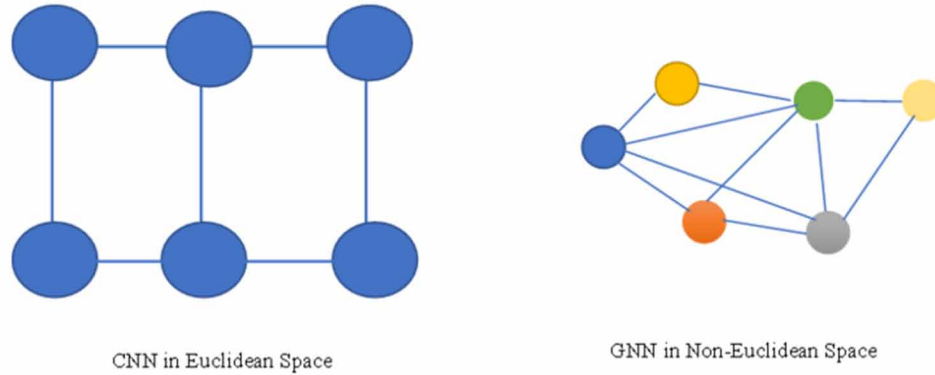
## CHALLENGES IN GRAPH LEARNING

Despite the recent success of (GNNs), still several challenges that need to be addressed for GNNs to be more effective and efficient. Here are some of the key challenges in GNN research:

- **Scalability:** The difficulty of scaling GNNs to larger and larger graphs is a significant obstacle. GNNs require computing node representations by aggregating information from their neighbors, which can be computationally expensive for large graphs with millions or billions of nodes. Developing scalable GNN architectures that can handle large-scale graphs is an active area of research.



Figure 2. CNN and GNN in Euclidean and non-Euclidean space



- **Generalization:** GNNs often struggle to generalize well to unseen graphs, especially when the graphs have different sizes, structures, and labels. This is because GNNs are sensitive to the local topology of the graph, node representations can be impacted prominently with the change of graph structure. Developing GNN architectures that can generalize well to unseen graphs is an important research direction.
- **Overfitting:** GNNs are prone to overfitting, especially when the graphs labeled nodes with limited numbers or with the noisy or sparse graph topology. This is because GNNs tend to learn the specific characteristics of the training graph, rather than the general graph properties. Developing regularization techniques and data augmentation strategies to prevent overfitting is an active area of research.
- **Interpretability:** GNNs are often considered as black-box models, making it challenging to interpret their predictions and understand how they make decisions. Developing interpretable GNN architectures that can provide insights into the graph structure and the learned representations is an important research direction.
- **Data Efficiency:** Due to the unavailability of sufficient data which can be a challenge in domains where labeled data is scarce or expensive to obtain, the GNN performance can drop. Developing GNN architectures that can learn from limited labeled data or transfer knowledge from related tasks is an active area of research.
- **Temporal Graph:** The first modeling challenge in graph neural network is temporal graph. For example, in social network the relation between node changes over the time. The connection between nodes depends on user actions and this is not predictable all the time. Different applications of identifying fraud like fraud credit card detection or other suspicious activity that affects the usual activity of the user. The graph model of deep neural network should respond to these changes and adapt to the new environment with the time. The main intention is to check how the algorithm responds to this kind of situation many problems.

Overall, addressing these challenges is crucial for the development of more effective and efficient GNNs, and for unlocking the full potential of GNNs in various domains.

## APPLICATIONS OF GRAPH NEURAL NETWORK

The challenges that a GNN can solve are divided into three categories:

1. **Classification of Node:** Predicting each node's embedding in a network is known as node classification of a node in a GNN. Based on the property of other nodes GNN (Liu & Zhou, 2020) can classify a new node. Here algorithm needs to determine the labelling sample of a node based on its neighbors. This type of approach is used in YouTube recommendations, Facebook friend recommendations etc.
2. **Predicting Link:** Predicting connection between two nodes or objects is the main aim of link prediction. For example, consider a recommendation system were based on user reviews model will create preferences for the user. Reviews with positive outcome will encourage highly to the user based on the link prediction of more similar kind of reviews.
3. **Graph Classification:** Classifying graph is one of the types of organizing similar kind of data items together. The main aim here is to classify the graph using certain graph (Xu et al., 2018) statistics which are like each other. For example, in a protein data graph classification can be useful to categorize chemical properties for the compounds of the protein.

## REAL-TIME APPLICATIONS OF GNN

Numerous fields and activities relying on graph-structured data (Zhou et al., 2018) have found success with the use of Graph Neural Networks (GNNs) (Velickovic et al., 2018). Some of the key applications of GNNs are described below:

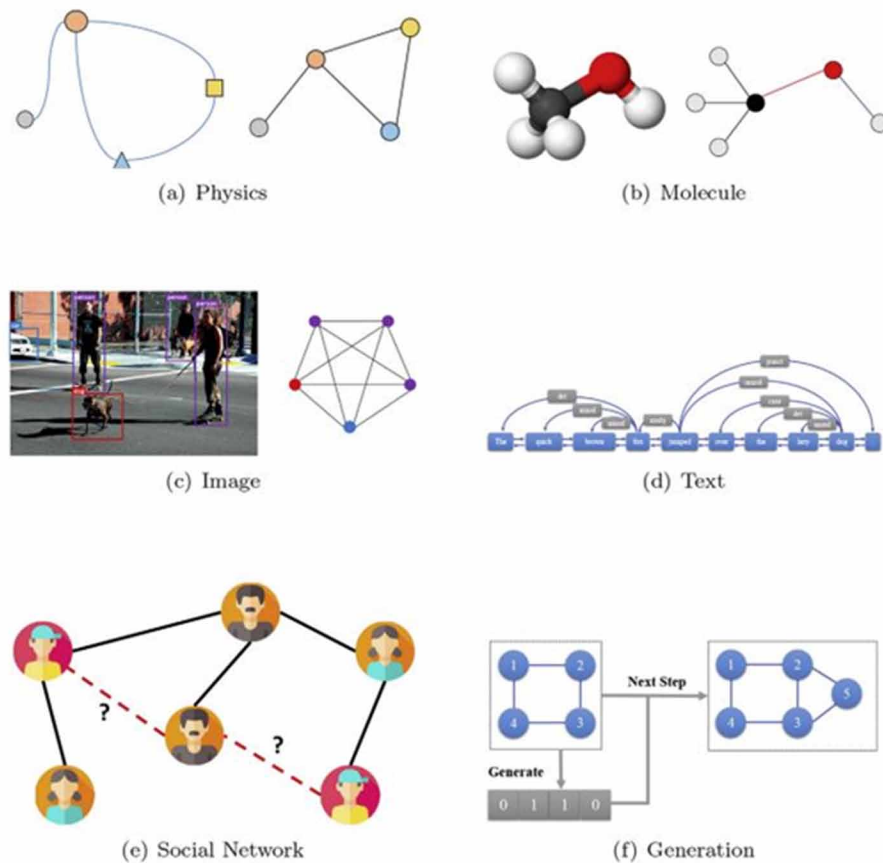
1. **Social Network Analysis:** GNNs have been used to model social networks and analyze their properties, such as drug community detection, link prediction, and influence maximization. GNNs can capture the complex relationships and interactions between individuals in social networks and enable more accurate predictions and recommendations.
2. **Drug Discovery:** GNNs have been used to design new drugs and predict their properties, such as toxicity and efficacy. GNNs can learn the molecular structure of compounds and predict their interactions with target proteins, enabling more efficient and cost-effective drug discovery.
3. **Recommendation Systems:** GNNs have been used to develop recommendation systems that can suggest relevant items or products to users based on their past behavior or preferences. GNNs can model the user-item interactions and the underlying graph structure of the recommendation network, enabling more accurate and personalized recommendations.
4. **Natural Language Processing:** GNNs have been used to model text data and perform tasks such as sentiment analysis, named entity recognition, and text classification (Li et al., 2016). GNNs can capture the syntactic and semantic relationships between words and sentences, enabling more accurate and contextualized text analysis.
5. **Finance:** GNNs have been used to model financial data and perform tasks such as fraud detection, risk assessment, and portfolio optimization. GNNs can capture the complex relationships and dependencies between financial assets, enabling more accurate and timely predictions.

## Graph Neural Network and Its Applications

6. **Computer Vision:** In the recent past year's computer vision has growth rapidly due to the significant growth of deep learning specially in image processing. Convolutional Neural Networks are a commonly utilized technique in deep learning. GNN is also widely used in the area of image processing (Vasudevan et al., 2022). GNN shows a great potential in the field of computer vision as things are emerging in this field more in the near future.
7. **Science:** Different scientific disease prediction and drug classification is one of the most useful applications of GNN. The drug chemical compound and atomic structure can be represented in the form of graph. Through this prediction and classification of drug for individual patient can be advised.
8. **Image Classification:** GNN along with convolution operation can be featured as graph convolution network. This is predominately used in image classification. GNN is to be considered to increase performance when there is a large training dataset. Graphs may be used to depict images by connecting the values of adjacent pixels that occur often together.

Figure 3. Different application areas of GNN

Source: Liu and Zhou (2020)



Overall, GNNs have shown promising results in various domains and tasks that involve graph-structured data and are expected to have a significant impact in many fields in the future.

## CURRENT TREND IN GRAPH NEURAL NETWORK

The current trend in Graph Neural Networks (GNNs) (Velickovic et al., 2019) is focused on developing more advanced and efficient architectures for modeling graph-structured data. Here are some of the key trends in GNN research:

**Graph Attention Networks (GATs):** As a subset of GNNs (Wu et al., 2020), GATs take use of attention processes to give neighboring nodes varied weights depending on their relative relevance in the graph. Because of this, the model may zero down on the most relevant information in the graph while disregarding the rest. Results from the use of GATs in a variety of tasks, including node classification, link prediction, and graph clustering, have been rather encouraging.

**Transformer-Based GNNs:** GNNs (Bronstein et al., 2017) now make use of the Transformer architecture, which was first suggested for use in NLP. To capture long-range relationships and global structures in the graph, Transformer-based GNNs employ self-attention methods to calculate node embeddings. State-of-the-art performance has been reached in applications like graph classification and node classification using transformer based GNNs.

**Hierarchical GNNs:** By combining data from various nodes in the graph's structure (Ye et al., 2022), hierarchical GNNs may more effectively learn representations at varying degrees of detail. This allows the model to accurately represent the graph's structure (Kumar et al., 2022) at both the micro and macro levels. In applications like graph classification and node classification, hierarchical GNNs have performed well.

**Graph Generative Models:** To create new graphs with properties identical to the input graphs, GNNs have also been utilized in graph generative models. Drug research and molecule design are only two examples of the many possible uses for the graph generative models (Biswas et al., 2021). Generating new compounds with the necessary characteristics using GNN-based graph generative models has demonstrated encouraging results.

**Graph Representation Learning:** In addition to its utility in node classification and link prediction, GNNs are also used in learning graph representations. Graph autoencoders, contrastive learning (Yadav et al., 2023), and other unsupervised and self-supervised methods have been suggested for learning graph representations.

GNN research focuses heavily on improved architectures for modelling graph-structured data, which is finding pervasive application in fields as divergent as computer vision, natural language processing, drug development, and social network analysis.

## FUTURE RESEARCH DIRECTIONS

One potential future direction for GNNs is their integration with reinforcement learning (RL). RL is a type of machine learning where an agent learns to interact with an environment to maximize a reward signal. GNNs could be used to represent the state of the environment, and the agent could use this representation to make decisions about which actions to take.

This integration of GNNs and RL has already been explored in some applications, such as robotics and game playing. However, there is still much research to be done in this area, including the development of more effective GNN architectures for RL and the exploration of new applications. Graph neural network have wide possibility in near future and as the growing era of deep learning its popularity is also increasing. In real scenario most of the data are mobile in nature and GNN can analyze these types of data very effectively. It may be recommendation system, image processing or personalized medicine recommendation almost all sector GNN have its functionality.

## **SUMMARY**

This chapter's conclusion on Graph Neural Networks (GNNs) emphasizes the bright future of this research field. GNNs have already demonstrated tremendous success in several applications, including computer vision, natural language processing, and drug discovery.

As GNNs continue to evolve, it is likely that they will be used in even more diverse applications and integrated with other areas of machine learning, such as reinforcement learning. To maximize a reward signal, agents trained using reinforcement learning learn to manipulate their environments. GNNs could be used to represent the state of the environment, and the agent could use this representation to make decisions about which actions to take. This integration of GNNs and reinforcement learning has already been explored in some applications, such as robotics and game playing. However, there is still much research to be done in this area, including the development of more effective GNN architectures for reinforcement learning and the exploration of new applications.

Future research in GNNs will likely focus on developing more effective architectures, exploring new applications, and improving our understanding of how GNNs learn and represent information. As this research progresses, GNNs are poised to become an increasingly important tool for solving complex problems in a variety of fields. In conclusion, Graph Neural Networks are an exciting new research frontier that will have long-term, far-reaching consequences for the whole discipline of machine learning.

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## **KEY TERMS AND DEFINITIONS**

**Graph Convolution Neural Network (GCNN):** Combining graph features with neural network where convolution neural network is not sufficient.

**Image Processing:** Getting useful information from the image and can be used in image classification and recognition.

**Node Embedding:** A node in a graph can extract information from another node if they are connected through similarity or any other condition.



## Chapter 3

# Introduction to Graph Neural Network: Types and Applications

**Ganga Devi S. V. S.**

*Madanapalle Institute of Technology and Science, India*

### **ABSTRACT**

*Deep learning on graphs is an upcoming area of study. This chapter provides an introduction to graph neural networks (GNNs), a type of neural network that is designed to process data represented in the form of graphs. First, it summarizes the explanation of deep learning on graphs. The fundamental concepts of graph neural networks, as well as GNN theories, are then explained. In this chapter, different types of graph neural network (GNN) are also explained. At the end, the applications of graph neural network where GNN is used and for what purpose it is going to be used are explained. This also explores the various applications of GNNs in fields such as social network analysis, recommendation systems, drug discovery, computer vision, and natural language processing. With the increasing prevalence of graph data, GNNs are becoming increasingly important and will likely continue to play a significant role in many fields in the future.*

### **INTRODUCTION**

A concise and interesting lesson on the key ideas and building blocks involved in neural networks for graphs is provided by researchers from the University of Pisa in Italy. Graph networks (Gori et al., 2005) are frequently used in the social sciences to describe the connections between individuals. For instance, they are used to represent the molecular structure of a drug, protein interaction networks, as well as biological and biochemical relationships in chemistry and material sciences. Graphs, in general, are an effective representational tool for rich and complicated data generated by a range of artificial and natural processes. A graph can be thought of as a structured datatype with nodes and edges that is relational and compositional in nature. Recent interest in deep learning models that can handle graphs in an adaptable

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way is increased due to the amount of information carried by such data and the growing accessibility of enormous repositories. The field of deep learning for graphs has its roots in early 1990s research on recursive neural networks (RecNN) for tree-structured data and neural networks for graphs. Later, the RecNN method was rediscovered in relation to applications for natural language processing. It was first applied to directed acyclic graphs and has since been generalized to more intricate and varied forms. Similar to the RecNN, the GNN model is based on a state transition system but allows for cycles in state computation. Therefore, the development of deep learning models that automatically extract the necessary features from a graph can be the focus of research. Deep Graph Networks are the name given to these models (DGNs). The authors classify deep graph networks (DGNs) into three main groups: deep neural graph networks (DNGNs) which include models based on neural architectures; deep Bayesian graph networks (DBGNs) whose representatives are probabilistic models of graphs and deep generative graph networks (DGGNs) which include generative approaches to graphs that may include both neural and probabilistic models.

## **Graph Neural Network (GNN)**

Data structures called graphs are used to simulate difficult real-world issues. Learning chemical fingerprints, simulating physical systems, managing traffic networks and friend recommendations on social media are few examples. While classic deep learning models such as Convolutional Neural Networks (CNNs) or Recurrent Neural Networks (RNNs) are not well suited to handle these tasks, they do require dealing with non-Euclidean graph data that contains rich relational information between nodes. The graph neural network is useful in this situation.

A deep learning neural network that is graph-structured is called a “graph neural network.” It can be compared to a graph where the nodes represent the data to be analyzed and the edges represent the connections between them. Conceptually, GNNs are built on deep learning and graph theory. A group of models has known as graph neural networks use graph representations to learn data structures and graph-related tasks (Kumar & Thakur, 2017). In order to acquire better representations on graphs via feature propagation and aggregation, graph neural networks (GNNs) are offered as a way to merge feature information and the graph structure.

Bronstein et al. (2017) provide an overview of deep learning techniques for non-Euclidean domains, such as graphs and manifolds, under the title geometric deep learning. Despite being the initial review of GNNs, this article focuses mostly on convolutional GNNs. A small selection of GNNs are covered by Hamilton et al. (2017) who concentrate on finding a solution to the network embedding issue. In comprehensive analysis of GNNs, Battaglia et al. (2018) place graph networks as the fundamental components for learning from relational data, reviewing part of GNNs under a unified framework. A partial survey of GNNs using various attention mechanisms is carried out by Lee et al. (2019).

## **Advantages**

Graph Neural Networks have a number of advantages over regular neural networks:

- GNNs may be trained on any dataset that has both input data and pairwise relationships between items. An important advantage graph neural networks have over regular deep learning is that graph neural networks are able to capture the graph structure of data – which is often very rich.

## ***Introduction to Graph Neural Network***

- GNNs can be used to classify data or make predictions.
- GNNs have a lot better memory footprint than regular deep learning models since they only need to store information about connections between nodes instead of all neurons in the graph.
- GNNs are very easy to train even with smaller datasets.

## **THEORIES OF GRAPH NEURAL NETWORKS**

Graph Neural Networks (Scarselli, et al., 2008) have a selection of the emerging theoretical results on approximation and learning properties of widely used message passing GNNs and higher-order GNNs, focusing on representation, generalization and extrapolation.

- **Representational Power of GNNs**

Here, how many neurons and training parameters a neural network has to have in order to approximate multivariate functions is examined. We can dispel the dimensionality curse by establishing upper constraints on these quantities for shallow and deep neural networks. Additionally, we demonstrate that the limitations almost exactly match the bare minimum of parameters that any continuous function approximator need to approximate Korobov functions, demonstrating that neural networks are almost the best function approximators.

- **Generalization**

The generalization capacity of GNNs on Out-Of-Distribution (OOD) circumstances as well as the agnostic distribution alterations between training and testing graphs are not considered when Graph Neural Networks are proposed. In this situation, even though there is a fake connection, GNNs often use the training sets subtle statistical correlations to make predictions. The failure of GNNs could result from such erroneous correlations change in testing conditions. For stable GNNs, it is essential to reduce the impact of spurious correlations. In order to do this, Stable GNN, a generic casual representation framework, extraction of high-level representations from graph data is the main concept.

In particular, a graph pooling layer is used to extract high-level representations based on subgraphs. The effectiveness, adaptability, and interpretability of the proposed framework have been thoroughly tested using synthetic and real-world OOD graph datasets.

- **Extrapolation**

While feedforward neural networks, also known as multilayer perceptrons (MLPs), do not extrapolate well in some simple tasks, Graph Neural Networks (GNNs)- structured networks with MLP modules- have shown some success in more complex tasks. MLPs and GNNs extrapolate effectively. First, we quantify the finding that ReLU MLPs quickly converge to linear functions in any direction from the origin suggesting that most nonlinear functions cannot be extrapolated by ReLU MLPs. However, if the training distribution is sufficiently diverse, they can provably learn a linear target function.

Second, these results point to a hypothesis that we support with theoretical and empirical data in relation to analyzing the successes and shortcomings of GNNs: the ability of GNNs to extrapolate al-

gorithmic tasks to new data (such as larger graphs or edge weights) depends on encoding task-specific non-linearities in the architecture or features.

## Types of Graph Neural Networks

The graph neural networks are categorized into different types, there are:

- Recurrent Graph Neural Networks (RecGNNs)
- Convolutional Graph Neural Networks (ConvGNNs)
- Graph Auto Encoders (GAEs)
- Spatial-Temporal Graph Neural Networks (STGNNs)

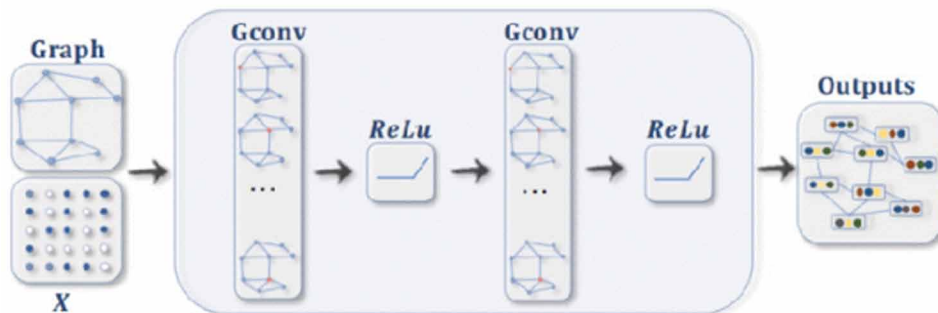
## Recurrent Graph Neural Networks

Most pioneering studies of graph neural networks are recurrent graph neural networks (RecGNNs). RecGNNs use recurrent neural networks to learn node representations. They assume that each node in a network communicates with each of its neighbors continuously until a stable equilibrium is attained. Conceptually significant RecGNNs served as an inspiration for later research on convolutional graph neural networks. In particular, spatial-based convolutional graph neural networks inherit the concept of message transmission.

## Convolutional Graph Neural Networks

Convolutional Graph Neural Networks (ConvGNNs) generalize the operation of convolution from grid data to graph data. The fundamental concept is to produce a node  $v$ 's representation by aggregating its own features and those of its neighbors, where  $u \in N(v)$ . ConvGNNs stack numerous graph convolutional layers to extract high-level node representations in contrast to RecGNNs. Figure 1 and Figure 2 shows a ConvGNN for node classification and graph classification respectively (Wu et al., 2020).

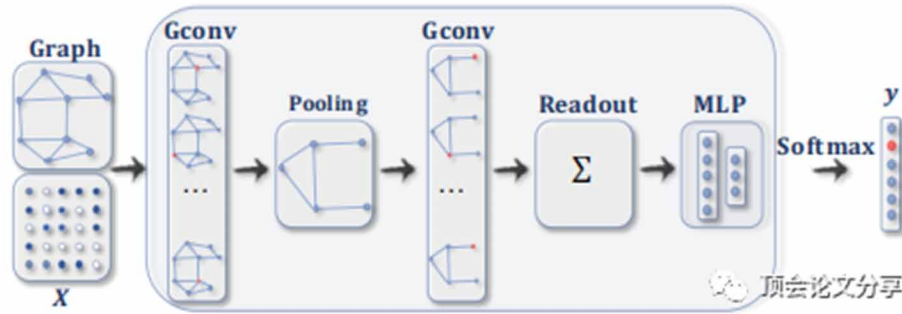
Figure 1. Multiple graph convolutional layers in a ConvGNN



## Introduction to Graph Neural Network

A graph convolutional layer encapsulates each node's hidden representation by aggregating feature information from its neighbors and a non-linear transformation is applied to the outputs. By stacking multiple layers, the final hidden representation of each node receives messages from a further neighborhood (Wu et al., 2020).

Figure 2. ConvGNN with pooling and readout layers for graph classification

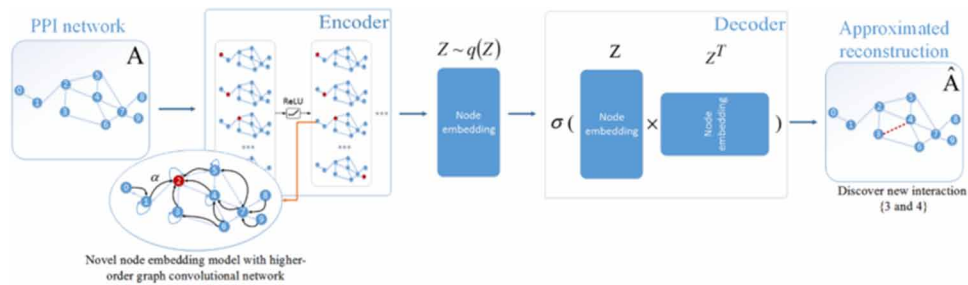


A graph convolution layer is followed by a pooling layer to coarsen a graph into subgraphs. A readout layer summarizes the final graph representation by taking sum/mean of hidden representations of subgraphs (Wu et al., 2020).

## Graph Auto Encoders

Unsupervised learning frameworks called “graph auto encoders” (GAEs) encode nodes or graphs into a latent vector space and reconstruct graph data from the encoded information. GAEs learn latent node representations through reconstructing graph structural information as the adjacency matrix. For graph generation, some methods generate nodes and edges of graph step by step, others generate all at once. Figure 3 shows a GAE for network embedding (Wu et al., 2020).

Figure 3. GAE for Network embedding

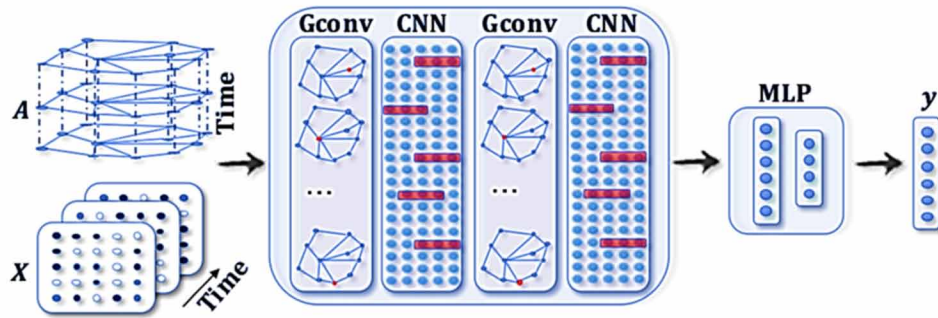


The encoder uses graph convolution layers to get a network embedding for each node. The decoder computes the pairwise distance given network embedding. A non-linear activation function is applied. The decoder reconstructs the adjacency matrix. The network is trained by minimizing the discrepancy between actual adjacency matrix and reconstructed adjacency matrix (Wu et al., 2020).

## Spatial-Temporal Graph Neural Networks

The goal of spatial-temporal graph neural networks (STGNNs) is to learn hidden patterns from spatial-temporal graphs. These patterns are significant for applications like predicting traffic speed (Li, et al., 2017), anticipating driver maneuvers (Jain et al., 2016) and human action recognition (Yan et al., 2018). The fundamental principle of STGNNs is to take both spatial and temporal dependency at same time. Many recent methods integrate graph convolutions to capture spatial dependency with RNNs or CNNs to model the temporal dependency. A STGNN for forecasting spatial-temporal graphs is shown in Figure 4.

Figure 4. A STGNN for forecasting spatial-temporal graphs



A graph convolutional layer is followed by a 1D-CNN layer. 1D-CNN layer slides over  $X$  along the time axis to capture the temporal dependency, while the graph convolutional layer operates on  $A$  and  $X(t)$  to capture the spatial dependency. A linear transformation is used in the output layer to produce a prediction for each node, such as future value at the next time step (Wu et al., 2020).

## Frameworks of GNN

GNN can focus on different graph analytics tasks.

- **Node-Level**

Tasks involving node classification and node regression are related to node-level outputs. RecGNNs and ConvGNNs can extract high level node representation by graph convolution. GNNs able to do node-level tasks in an end-to-end manner with a multi-perceptron or a softmax layer as the output layer.

- **Edge-Level**

This output relates to the edge classification and link prediction tasks. A similarity function or neural network may be used to estimate the label/connection strength of an edge given the hidden representations of two nodes from GNNs.

- **Graph-Level**

Graph-level outputs relate to the Graph classification problem. GNNs are frequently used with pooling and readout operations to get a compact representation at the graph level.

GNNs can be trained in a (semi) supervised or Un supervised way within an end to end learning framework, depending on the learning tasks and label information available.

## APPLICATIONS OF GRAPH NEURAL NETWORKS

The problems that GNNs resolve can be classified into these categories:

1. **Node Classification:** Here, the aim is to identify the labeling of samples (shown as nodes) by examining their neighbours labels. This kind of problem is typically taught semi-supervised with only a portion of the graph labeled.
2. **Graph Classification:** Sorting the entire graph into separate groups is the task at hand. The focus shifts to the graph domain similar to picture categorization. Graph classification has several uses, includes detecting whether or not a protein is an enzyme in bioinformatics, classifying articles in natural language processing and social network analysis.
3. **Graph Visualization:** At the nexus of geometric graph theory and information visualization, it is a field of mathematics and computer science. It is focused with the visual depiction of graphs that helps the user comprehend the graphs by revealing structures and abnormalities that may be present in the data.
4. **Link Prediction:** Here, the algorithm must comprehend how entities interact in graphs and attempt to foretell whether two entities will be connected. Inferring social relationships or recommending potential buddies to users is crucial in social networks. It has also been applied to problems with recommender systems and the identification of criminal links.
5. **Graph Clustering:** It alludes to the graph-based clustering of data. On graph data, clustering is done in two different ways. By using edge weights or edge distances, vertex clustering attempts to group the graph's nodes into densely connected clusters. The second method of clustering graphs does so by treating the graphs as the items to be grouped and group them based on similarity.

Let's go through some applications across domains where GNN can resolve various challenges.

## **GNNs IN COMPUTER VISION**

Machines can differentiate and identify objects in pictures and movies using standard CNNs. However, much work needs to be done before machines can exhibit human-like visual intuition. GNN architectures, however, can be used to solve image categorization issues.

One of these issues is scene graph generation where the model attempts to separate an image into an object-and-relationship semantic network. Scene graph generation models can identify things in an image and foretell the semantic links that exist between them when they are paired.

GNNs are still being used in a rising number of computer vision applications, nevertheless. It also includes things like human-object interaction and few-shot picture classification.

## **GNNs in Natural Language Processing**

According to NLP, text is a kind of sequential data that can be characterized by an RNN or an LSTM. However, because they are so natural and simple to express, graphs are frequently employed in numerous NLP tasks.

The use of GNNs for numerous NLP issues, including text classification, utilizing semantics in machine translation, user geolocation, relation extraction, and question answering, has seen a recent uptick in interest.

Every node is recognized as a separate entity, and edges define the connections between them. The issue of question answering has long existed in NLP research. However, it was constrained by the current database. Although the methodology can be extended to previously undiscovered nodes using tools like GraphSage.

## **GNNs in Traffic**

A key component of a smart transportation system is the ability to forecast traffic volume, speed, or road density. Utilizing STGNNs, we can solve the traffic forecast issue (Spatial-Temporal Graph Neural Networks).

Imagine the traffic network as a spatial-temporal graph, with nodes representing the sensors placed on roadways, edges representing the separation between pairs of nodes, and dynamic input features representing the average traffic speed within a window for each node (Li et al., 2017).

## **GNNs in Chemistry**

GNNs can be used by chemists to investigate the graph structure of molecules or substances. Atoms serve as nodes and chemical bonds serve as edges in these graphs.

## **GNNs in Other Domains**

GNNs can be used for more than only the tasks and domains listed above. Program verification, program reasoning, social influence prediction, recommender systems, electrical health records modeling, brain networks, and adversarial attack prevention are just a few of the issues to which GNNs have been attempted to be used (Ying et al., 2018).



## **Future Directions of GNNs**

Despite GNNs' success in learning graph data, difficulties still persist because of the complexity of graphs. Here four potential avenues for GNN development are outlined in this section.

### **Model Depth**

Deep neural architectures are key to deep learning's success (He et al., 2016). However, Li et al. (2018) demonstrate that when the number of graph convolutional layer increases, the performance of a ConvGNN declines significantly. Theoretically, with an infinite number of graph convolutional layers, all nodes' representations will converge to a single point because graph convolutions move the representations of nearby nodes closer to one another (Li et al., 2018). This prompts the query of whether learning graph data by diving deep is still a sound methodology (Kumar & Thakur, 2018).

### **Scalability Trade-Off**

The completeness of the graph is compromised in exchange for the scalability of GNNs. A model will lose some of the information about the graph whether sampling or clustering is used. A node risks missing its important neighbors through sampling. A graph may lose its distinctive structural pattern as a result of clustering. Future study may focus on how to balance graph integrity and algorithm scalability.

### **Heterogeneity**

Most modern GNNs assume that graphs are homogeneous. It is challenging to apply directly current GNNs to heterogeneous graphs, which may include various node and edge types as well as various node and edge inputs, such as text and images. Therefore, new techniques for dealing with diverse graphs should be created.

### **Dynamicity**

Graphs by their very nature are dynamic, with nodes and edges that can alter over time as well as their inputs. For graphs to adapt to their dynamic nature, new graph convolutions are required. Although STGNNs can partially handle the dynamic nature of graphs, few of them consider how to conduct graph convolutions in the context of dynamic spatial relations.

## **CONCLUSION**

In conclusion, Graph Neural Networks (GNNs) have emerged as a powerful tool for analyzing and processing complex, non-Euclidean data structures represented in the form of graphs. The different types of GNNs such as Graph Convolutional Networks (GCNs), Graph Attention Networks (GATs), Graph Autoencoders (GAEs), and Graph Generative Models have their own strengths and are suitable for different applications. An overview of graph neural networks was taken in this study. Recurrent graph neural networks, convolutional graph neural networks, graph autoencoders, and spatial-temporal graph

neural networks are the four categories divided in graph neural networks. GNNs have found wide applications in various fields such as social network analysis, recommendation systems, drug discovery, computer vision, and natural language processing. As more and more data is being represented in the form of graphs, GNNs are becoming increasingly important and will likely continue to play a significant role in many fields in the future.

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# Chapter 4

## Graph Classification of Graph Neural Networks

**Gotam Singh Lalotra**

*Government Degree College, Basohli, India*

**Ashok Sharma**

*University of Jammu, India*

**Barun Kumar Bhatti**

*Government Degree College for Women, Kathua, India*

**Suresh Singh**

*GGM Science College, Jammu, India*

### ABSTRACT

*Graph neural networks have recently come to the fore as the top machine learning architecture for supervised learning using graph and relational data. An overview of GNNs for graph classification (i.e., GNNs that learn a graph level output) is provided in this chapter as pooling layers, or layers that learn graph-level representations from node-level representations, are essential elements for successful graph classification because GNNs compute node-level representations. Hence, the authors give a thorough overview of pooling layers. The constraints of GNNs for graph categorization are further discussed, along with developments made in overcoming them. Finally, they review some GNN applications for graph classification and give an overview of benchmark datasets for empirical analysis.*

### INTRODUCTION

In mathematics and computer science, a graph is a collection of vertices (also known as nodes) and edges that connect pairs of vertices. Graphs are widely used to model and represent relationships and connections between different entities, such as people in a social network, web pages on the internet, or molecules in a chemical compound (Trudeau, 2013). Graph classification is the task of predicting a single label for an entire graph. In recent years, Graph Neural Networks (GNNs) have emerged as a powerful approach

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for graph classification. A graph is typically represented visually as a set of points (vertices) and lines (edges) connecting them (Kumar & Thakur, 2017). Each edge represents a relationship between two vertices, and may have a direction or be undirected. A directed edge connects two vertices in a specific direction, while an undirected edge connects two vertices in both directions. There are many different types of graphs, including directed graphs, undirected graphs, weighted graphs, and bipartite graphs. Directed graphs have edges with a direction, while undirected graphs have edges without a direction. Weighted graphs have a value assigned to each edge, which can represent attributes such as distance, cost, or strength. Bipartite graphs are a type of graph where the vertices can be divided into two disjoint sets, and all edges connect vertices from one set to the other.

Graphs have a wide range of applications in various fields, including computer science, mathematics, physics, and biology. They are used in algorithms for shortest path problems, network flow, and clustering. Graph databases are used to store and analyze large-scale data, while graph theory is used to study properties of graphs and their applications.

GNNs are deep learning models that operate directly on graphs, and they can learn to extract features and make predictions for graphs of varying sizes and shapes. Since data from real-world applications have very diverse forms, from matrix and tensor to sequence and time series, a natural question that arises is why we attempt to represent data as graphs (Hamilton, 2020). Graphs, which describe pairwise relations between entities, are essential representations for real-world data from many different domains, including social science, linguistics, chemistry, biology, and physics. Graphs are widely utilized in social science to indicate the relations between individuals. In chemistry, chemical compounds are denoted as graphs with atoms as nodes and chemical bonds as edges (Bonchev, 1991). The basic idea behind GNNs is to propagate information between neighboring nodes in the graph. This is done by defining a neural network that takes as input the features of a node and its neighboring nodes, and produces an output that represents the updated features of the node. The updated features can then be propagated to its neighbors, and the process is repeated for several layers of the network. In this way, the GNN can learn to encode information about the local structure of the graph, as well as global information about the graph as a whole. In linguistics, graphs are utilized to capture the syntax and compositional structures of sentences. For example, parsing trees are leveraged to represent the syntactic structure of a sentence according to some context-free grammar, while Abstract Meaning Representation (AMR) encodes the meaning of a sentence as a rooted and directed graph (Banarescu et al., 2013). Hence, research on graphs has attracted immense attention from multiple disciplines.

Graph classification is a task in which a machine learning model is trained to predict the class labels of graphs. Graph neural networks (GNNs) are a popular class of models used for graph classification tasks. GNNs extend traditional neural networks to operate on graph-structured data, which makes them well-suited for tasks involving graphs, such as graph classification.

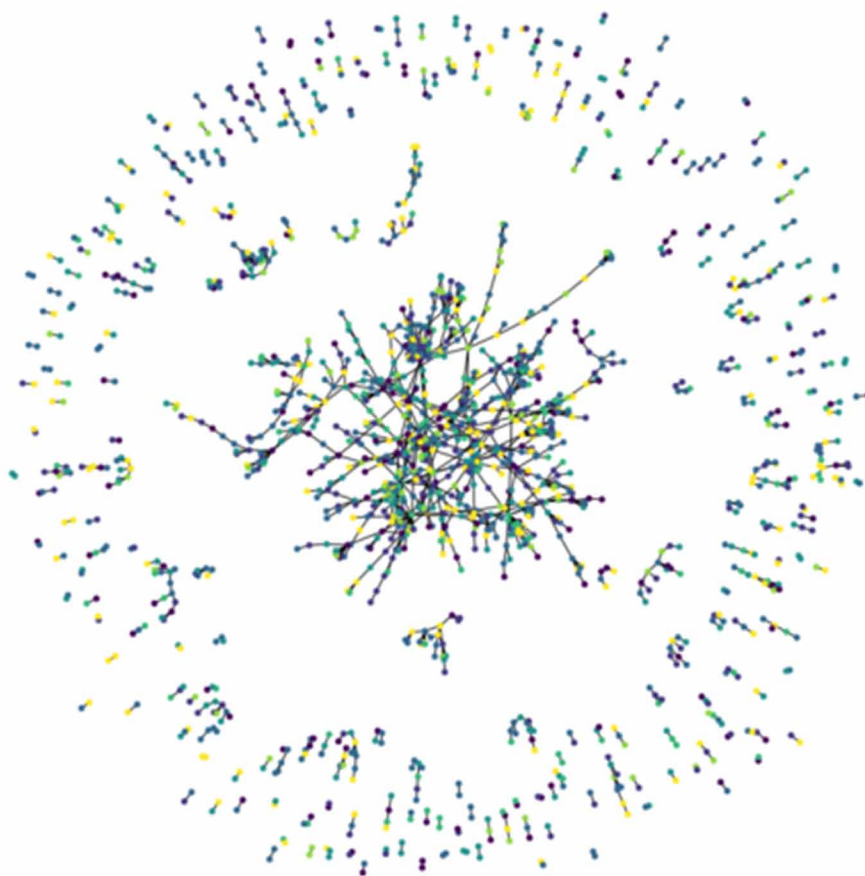
The basic idea behind GNNs is to learn node embeddings (i.e., low-dimensional representations of each node in the graph) that capture both local and global structural information of the graph. The node embeddings are updated iteratively by aggregating the embeddings of neighboring nodes and applying a neural network (Ziwei Zhang et al., 2015). There are many variations of GNNs, such as Graph Convolutional Networks (GCNs), Graph Attention Networks (GATs), and GraphSAGE, among others (Zhang et al., 2019). These models differ in how they update node embeddings and aggregate information across the graph (Lalotra et al., 2022). The classification of Graph Neural Networks (GNNs) is important because it allows researchers and practitioners to select the most appropriate GNN architecture and message-passing mechanism for a given task and graph data. Different types of graphs have unique characteristics and

## ***Graph Classification of Graph Neural Networks***

properties, and the appropriate GNN architecture and message-passing mechanism can vary depending on the type of graph data being processed. For example, a Graph Convolutional Network (GCN) might be a good choice for a task involving a homogeneous graph with a fixed neighborhood size, while a Graph Attention Network (GAT) might be more appropriate for a task involving a heterogeneous graph with variable neighborhood sizes.

Furthermore, different GNN architectures and message-passing mechanisms have different strengths and weaknesses in terms of scalability, memory efficiency, and interpretability. By understanding the different types of GNNs and their properties, researchers and practitioners can select the most appropriate GNN for their specific task and optimize its performance. Overall, the classification of GNNs provides a useful framework for understanding the different approaches to processing graph data and can help guide the development of more effective and efficient GNN models for a wide range of applications, including social network analysis, recommendation systems, and drug discovery. To perform graph classification, the final node embeddings are passed through a pooling layer that aggregates the node embeddings into a single graph embedding. This graph embedding is then fed into a fully connected neural network for classification.

*Figure 1. Graph classification*



Overall, GNNs have shown great success in graph classification tasks, outperforming traditional graph-based methods on several benchmarks. They have been applied to a wide range of domains, including chemistry, social networks, and biological networks.

## **BACKGROUND**

Graph classification is a challenging task in machine learning, and it has received increasing attention in recent years due to the proliferation of graph-structured data in various domains such as bioinformatics, social network analysis, and natural language processing. However, traditional machine learning approaches, such as kernel-based methods or decision trees, have limited capability in handling graph data with varying sizes and topologies. Graph Neural Networks (GNNs) were proposed as a way to directly learn representations of graph-structured data in a neural network framework. The first GNNs were introduced in the 2000s, but they gained wider attention in the last decade with the introduction of more powerful models such as Graph Convolutional Networks (GCNs) and Graph Attention Networks (GATs). GNNs are a type of neural network that is designed to operate on graph-structured data. They extend traditional neural networks by incorporating graph convolutional layers that aggregate information from neighboring nodes to update the node embeddings. In GCNs, the node features are updated by aggregating information from the features of its neighboring nodes using convolutional operations. This allows the model to learn both local and global features of the graph. In GATs, attention mechanisms are used to assign weights to the neighboring nodes based on their importance, which allows the model to focus on the most relevant nodes. GNNs have shown impressive performance in graph classification tasks, especially in domains such as bioinformatics where the input graphs are small and densely connected. They have also been used in other applications such as node classification, link prediction, and graph generation. However, challenges remain in scaling GNNs to handle larger and more complex graphs, as well as in dealing with noisy and incomplete data. The node embeddings are then passed through multiple layers of the neural network, allowing the model to capture both local and global structural information of the graph. GNNs have been successfully applied to various tasks involving graphs, such as node classification, link prediction, and graph classification.

## **GRAPH CLASSIFICATION WITH GNNs**

Graph classification with GNNs involves predicting the class labels of entire graphs, rather than individual nodes or links. The goal is to learn a function that maps a graph to its corresponding class label. The input to the model is a graph  $G = (V, E)$ , where  $V$  is the set of nodes and  $E$  is the set of edges, along with its associated features. The output is a class label  $y$ , which is a scalar value that indicates the class of the graph.

The first step in graph classification with GNNs is to compute node embeddings that capture the structural information of the graph (Wang et al., 2021). This is done by applying multiple layers of graph convolutional networks (GCNs) or other variants of GNNs, such as GraphSAGE or GATs. The node embeddings are updated iteratively by aggregating the embeddings of neighboring nodes and applying a neural network layer. The final node embeddings are then passed through a pooling layer that

## ***Graph Classification of Graph Neural Networks***

aggregates them into a single graph embedding. This graph embedding is then fed into a fully connected neural network for classification.

Graph Neural Networks (GNNs) can be classified based on their architecture, message-passing mechanism, and type of graph data they process. Some common classifications of GNNs are:

1. **Graph Convolutional Networks (GCNs):** GCNs use convolutional filters to aggregate information from neighboring nodes in a graph. They are feedforward networks that operate on fixed-size neighborhoods of nodes and can handle both directed and undirected graphs.
2. **Graph Attention Networks (GATs):** GATs use attention mechanisms to selectively focus on certain nodes or edges based on their importance or relevance to the task. They can handle both directed and undirected graphs and are particularly effective for graph classification and node classification tasks.
3. **Graph Recurrent Neural Networks (GRNNs):** GRNNs are recurrent networks that can handle sequential or temporal data on graphs. They operate on paths in the graph and can model long-term dependencies between nodes.
4. **Graph Isomorphism Networks (GINs):** GINs use a learnable permutation-invariant function to aggregate information from the entire graph. They are particularly effective for graph classification tasks and can handle both directed and undirected graphs.
5. **Message Passing Neural Networks (MPNNs):** MPNNs use a message-passing mechanism to propagate information between nodes in a graph. They can handle both directed and undirected graphs and are particularly effective for molecular property prediction and drug discovery.
6. **Graph Auto-Encoders (GAEs):** GAEs use an encoder-decoder architecture to learn a low-dimensional representation of the graph that can capture its structural and topological properties. They can handle both directed and undirected graphs and are particularly effective for graph reconstruction and link prediction tasks.

These are just a few examples of GNN classifications. Depending on the specific task and application, GNNs can be further classified based on additional criteria, such as their memory efficiency, scalability, or interpretability.

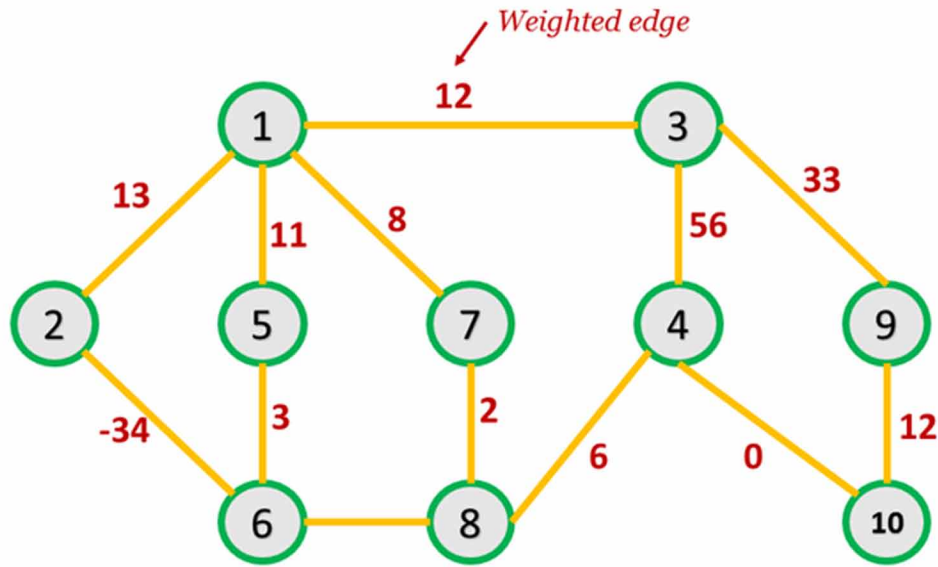
## **RECENT ADVANCES**

There have been several recent advances in GNNs for graph classification. One area of research is the development of more sophisticated pooling techniques that can better capture the global structural information of the graph. For example, some recent works have proposed using graph attention mechanisms to weight the contribution of each node to the graph embedding. Another area of research is the development of more efficient GNN architectures that can scale to large graphs. This is particularly important in applications such as social network analysis or biological networks, where the graphs can be extremely large. One recent work proposed using sparse matrix multiplication to speed up the computation of graph convolutional layers.

There have been several recent advances in Graph Classification of Graph Neural Networks (GNNs). Here are some of the notable ones:

1. **Incorporating Edge Information:** Recent research has shown that incorporating edge information can improve the performance of GNNs in graph classification tasks (Gong & Cheng, 2018). Some works have proposed methods to encode edge attributes and structural information in GNNs, allowing the model to capture more fine-grained information about the graph.

Figure 2. Weighted edge graph



## Weighted Edge Graph

Some common techniques for incorporating edge information in GNNs are:

- a. **Edge Features:** One straightforward way to incorporate edge information is to include additional features for each edge in the graph. These features can be added to the message passing step of the GNN, allowing the model to capture the interaction between nodes through their edges.
- b. **Edge Convolution:** Edge convolution involves convolving the edge features with learned filters and aggregating the resulting features with node features. Edge convolution can be used to capture the local edge structure around each node and model the interactions between neighboring nodes.
- c. **Edge Attention:** Edge attention involves learning attention weights for each edge, based on the features of its incident nodes. The attention weights can then be used to weight the message passing between nodes, allowing the model to focus on the most important edges for a given task.
- d. **Graph Attention:** Graph attention involves learning attention weights for each node and its edges, based on their features. The attention weights can then be used to weight the aggregation of node and edge features, allowing the model to focus on the most important nodes and edges for a given task.



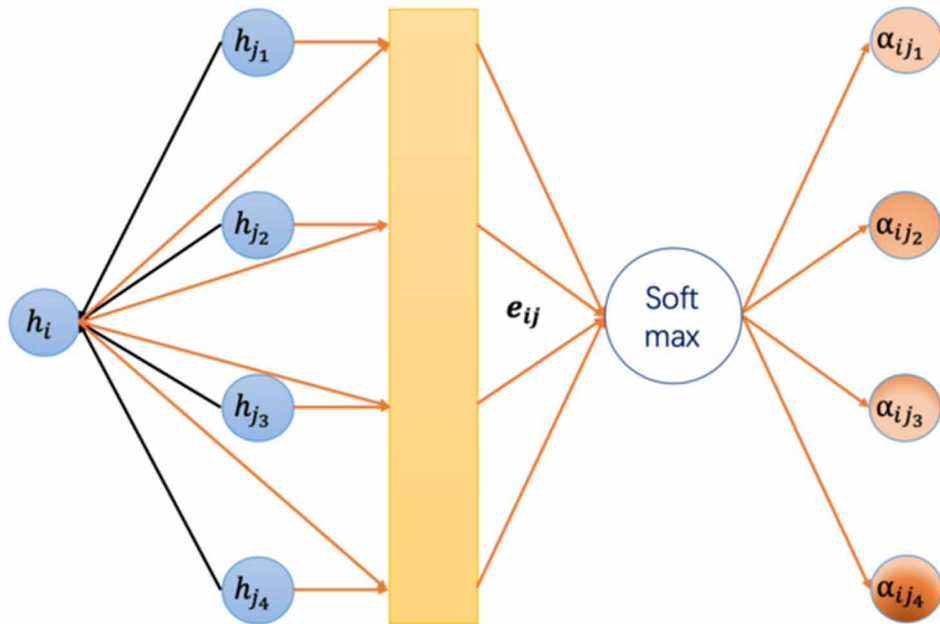
## Graph Classification of Graph Neural Networks

- e. **Graph Convolutional Networks (GCNs):** GCNs can be used to incorporate both node and edge information in a single framework. GCNs involve convolving both node and edge features using learned filters and aggregating the resulting features to update the node embeddings.

Incorporating edge information can be particularly useful in tasks such as link prediction, where the goal is to predict the presence or absence of edges between nodes. It can also be useful in tasks such as node classification or graph classification, where the interactions between nodes through their edges can provide valuable information for the task.

- 2. **Graph Attention Networks (GATs):** GATs are an extension of GCNs that incorporate attention mechanisms to allow the model to attend to different parts of the graph. Recent works have shown that GATs can achieve state-of-the-art performance in graph classification tasks, especially when the graph has a complex structure.

Figure 3. Graph attention network

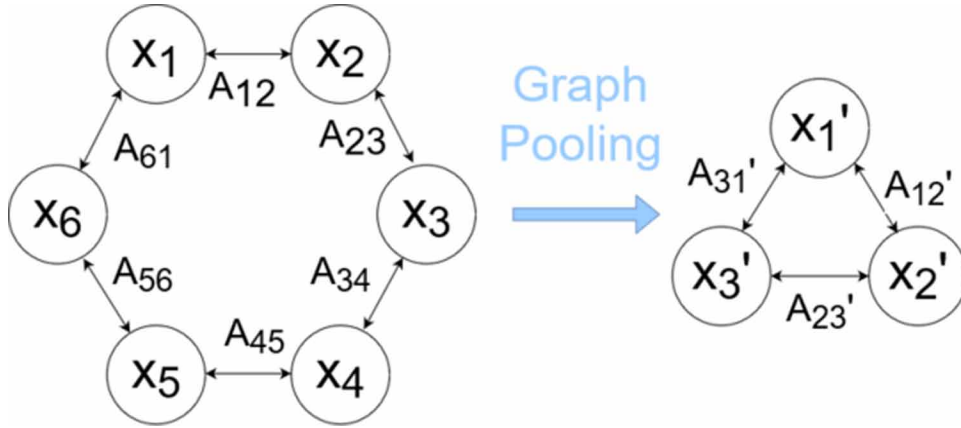


Graph Attention Networks (GATs) are a type of Graph Neural Network (GNN) that use attention mechanisms to weight the importance of each node's neighbors when aggregating information during the message passing process. The attention mechanism in GATs allows the model to learn a set of weights that specify how much attention should be paid to each neighbor of a given node. These weights are learned by optimizing the model's objective function during training. In GATs, the message passing process is done by computing a weighted sum of the features of each neighboring node, where the weights are obtained from the attention mechanism. The output of this process is then passed through a non-linear

activation function to obtain the final output of the node. One of the benefits of using GATs is that they are able to capture the local structure of the graph in a more flexible and expressive way compared to other GNN architectures, such as Graph Convolutional Networks (GCNs). This is because the attention mechanism in GATs allows each node to attend to its neighbors in a more fine-grained way, rather than treating all neighbors equally as in GCNs. Furthermore, GATs have shown state-of-the-art performance in various tasks, such as node classification and link prediction, on a wide range of datasets.

3. **Graph Pooling:** Graph pooling is an important step in GNN-based graph classification, which involves reducing the size of the graph by aggregating node embeddings (Gao & Ji, 2019). Recent works have proposed several advanced pooling techniques, including set-pooling, attention-based pooling, and hierarchical pooling, which have shown promising results in graph classification tasks.

Figure 4. Graph pooling



In GNNs, pooling is performed by grouping nodes together and aggregating their features to obtain a smaller set of nodes. This aggregation can be done using different methods, such as mean pooling, max pooling, or attention-based pooling. The resulting smaller graph can then be used as input for the next layer of the GNN. Graph pooling is particularly useful when dealing with large graphs, as it can reduce the computational cost of the GNN while still preserving important information about the graph structure. Additionally, pooling can help reduce overfitting in the GNN by removing redundant information and generalizing the learned features. There are several types of graph pooling methods used in GNNs, including:

- a. **Top-K Pooling:** This method selects the top-K nodes based on a certain criterion, such as their node degree, and aggregates their features to obtain a smaller set of nodes.
- b. **Diffusion Pooling:** This method propagates node features using a diffusion process, and selects a subset of nodes based on their final feature representations.
- c. **Coarsening Pooling:** This method aggregates nodes using a coarsening process, where the graph is successively simplified by merging nodes and edges until a desired size is reached.

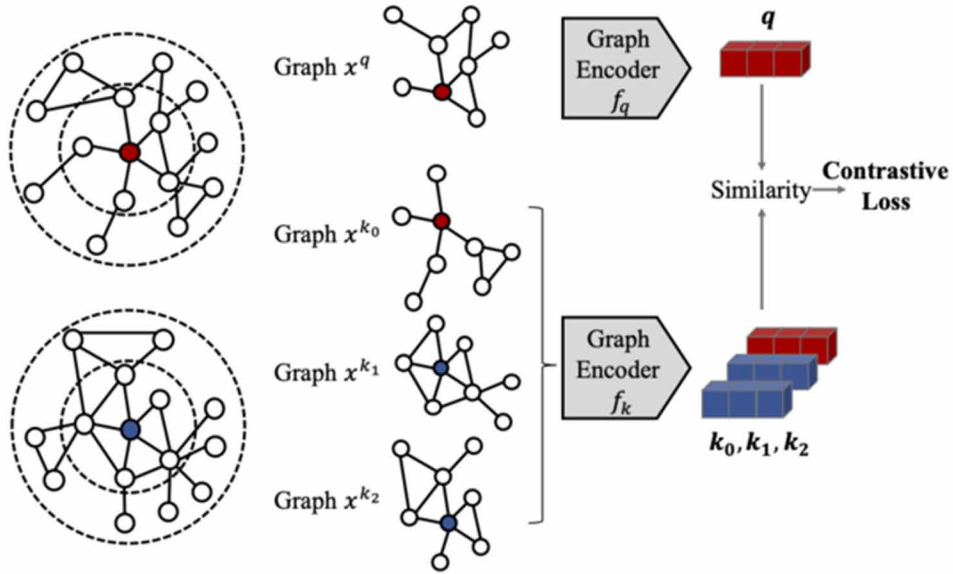
## Graph Classification of Graph Neural Networks

- d. **Attention Pooling:** This method uses an attention mechanism to weight the importance of each node, and aggregates their features based on their attention scores.

Overall, graph pooling is an important technique in GNNs for reducing the size and complexity of large graphs, while still retaining important structural information.

4. **Graph Contrastive Learning:** Contrastive learning is a popular method for unsupervised representation learning, which has recently been applied to graph classification. This approach involves training the model to distinguish between positive and negative pairs of graphs, where positive pairs are graphs that belong to the same class, and negative pairs are graphs from different classes. This approach has shown promising results in learning discriminative graph representations without requiring any labeled data.

Figure 5. Graph contrastive learning



Graph Contrastive Learning is a self-supervised learning method used in Graph Neural Networks (GNNs) to learn representations of nodes or subgraphs that are similar if they are semantically related and dissimilar otherwise. The objective of Graph Contrastive Learning is to maximize the similarity between positive pairs of nodes or subgraphs, while minimizing the similarity between negative pairs. The similarity between pairs is measured using a contrastive loss function that penalizes the distance between the representations of the nodes or subgraphs. In Graph Contrastive Learning, positive pairs are defined as pairs of nodes or subgraphs that are connected in the input graph or belong to the same class, while negative pairs are defined as pairs that are not connected or belong to different classes. By optimizing the contrastive loss function, the GNN is able to learn representations that capture the semantic similarity between nodes or subgraphs, which can then be used for downstream tasks such as node classification or link prediction. One advantage of Graph Contrastive Learning is that it does not

require labeled data, making it suitable for unsupervised learning tasks where labeled data is scarce. Additionally, Graph Contrastive Learning can be combined with other self-supervised or supervised learning methods to further improve the performance of the GNN.

Overall, Graph Contrastive Learning is an effective technique for learning representations of nodes or subgraphs in a self-supervised manner, and has shown promising results in various graph-related tasks.

5. **Graph Embedding Pre-Training:** Pre-training is a popular technique for learning useful representations of data that can be fine-tuned for downstream tasks. Recent works have proposed pre-training GNNs on large-scale graph datasets, such as Reddit or Wikipedia, and then fine-tuning them for graph classification tasks (You et al., 2020; Hu et al., 2019). This approach has shown significant improvements in the performance of GNNs on graph classification benchmarks.

Graph Embedding Pre-training is a technique used in Graph Neural Networks (GNNs) to learn meaningful representations of nodes or subgraphs by training a GNN on a large unlabeled graph dataset in a self-supervised manner. The learned representations can then be used as a starting point for downstream tasks such as node classification, link prediction, and graph clustering. The basic idea of Graph Embedding Pre-training is to pre-train a GNN on a large graph dataset using a self-supervised task, such as node attribute prediction or graph reconstruction, to learn node or subgraph representations. The learned representations can then be fine-tuned on a smaller labeled dataset for a specific downstream task. One of the key advantages of Graph Embedding Pre-training is that it allows the GNN to learn meaningful representations of nodes or subgraphs that capture the underlying graph structure and can be used across different tasks and datasets. Additionally, pre-training on a large graph dataset can help mitigate the problem of overfitting and improve the generalization ability of the GNN.

There are several pre-training methods used in Graph Embedding Pre-training, including:

- a. **Node-Level Pre-Training:** In this method, the GNN is trained to predict the attributes of individual nodes in the graph based on their neighborhood information.
- b. **Graph-Level Pre-Training:** In this method, the GNN is trained to reconstruct the original graph based on its node and edge features.
- c. **Context-Level Pre-Training:** In this method, the GNN is trained to predict the context of nodes or subgraphs based on their neighborhood information.

Graph Embedding Pre-training is a powerful technique for learning meaningful representations of nodes or subgraphs in a self-supervised manner, and has shown promising results in various graph-related tasks.

These advances have led to significant improvements in the performance of GNNs in various applications, such as drug discovery, social network analysis, and recommendation systems. Moreover, these developments have opened up new avenues for applying GNNs to a wider range of domains and tasks, and further progress is expected in the coming years. Overall, these recent advances in Graph Classification of Graph Neural Networks have significantly improved the performance of GNNs in various graph classification tasks, and further research in this area is expected to continue to advance the field.

## CHALLENGES WITH GNN

Notwithstanding the tremendous success that GNNs have had in numerous sectors, it is surprising that GNN models are not sufficient to produce satisfactory answers for each graph under any situation. There are, however, a few problems that will need to be fixed in the future.

### 1. Robustness

GNNs are a class of neural network-based models that are vulnerable to attacks. Unlike adversarial attacks on photos or text, which just focus on features, attacks on graphs take structure information into account. Existing graph models have been the target of several attacks (Zugner et al., 2018; Dai et al., 2018), and more durable models are being developed to defend them (Ji, 2019). Robustness in Graph Neural Networks (GNNs) refers to the ability of the model to maintain its performance when faced with various types of perturbations or changes to the input data, such as node or edge removal, noise, and attacks. There are different approaches to improving the robustness of GNNs, including:

- a. **Graph Augmentation:** This involves adding synthetic nodes or edges to the graph to increase its connectivity and enhance the model's ability to generalize to unseen data.
- b. **Adversarial Training:** This involves training the model on adversarial examples, which are modified versions of the input data designed to cause the model to make incorrect predictions. This can improve the model's ability to resist attacks and detect anomalous patterns in the data.
- c. **Dropout Regularization:** This involves randomly dropping out nodes or edges during training to reduce overfitting and improve the model's ability to generalize to new data.
- d. **Graph-Level Regularization:** This involves adding regularization terms to the loss function to encourage the model to learn more robust representations that are less sensitive to perturbations in the input data.

### 2. Interpretability

It is essential to apply GNN models to real-world applications with solid explanations. A few approaches provided example-level explanations (Chen et al., 2020; Baldassarre et al., 2019). Similar to the fields of CV and NLP, the issue of interpretability on graphs is one that needs to be thoroughly researched.

Interpretability in Graph Neural Networks (GNNs) refers to the ability to understand how the model arrives at its predictions or decisions. GNNs are often used for tasks such as node classification, link prediction, and graph classification, where the model needs to learn representations of the graph structure and its nodes/edges. Interpretability is important in applications where decisions made by the model need to be explained to humans or where transparency is required. For example, in drug discovery, it is important to understand why the model has predicted a certain molecule to have a particular biological activity.

There are different approaches to improving the interpretability of GNNs, including:

- a. **Visualization:** This involves plotting the graph structure and node embeddings to gain insights into how the model is representing the data.

- b. **Feature Attribution:** This involves calculating the contribution of each node or edge to the final prediction or decision, which can help to understand which parts of the graph are most important for the task.
- c. **Rule Extraction:** This involves extracting rules or patterns from the model that can be easily understood by humans.
- d. **Attention Mechanisms:** This involves using attention mechanisms to highlight important nodes or edges in the graph, which can help to understand which parts of the graph the model is focusing on.

Overall, improving the interpretability of GNNs is an active area of research and is important for building trust in these models and enabling their deployment in real-world applications.

### 3. Graph Pretraining

As collecting a lot of large-scale human-labeled data is expensive, neural network-based models require a lot of labelled data. Self-supervised techniques are provided to support models learn from unlabeled data available through websites or knowledge bases. These methods have achieved great success in the sectors of CV and NLP with the idea of pretraining (Devlin et al., 2018). Recent studies have looked into pretraining on graphs (Wang et al., 2020), but each of them has a unique issue setting and focuses on a different subject.

Graph pretraining is a powerful technique for training Graph Neural Networks (GNNs) that involves training a model on a large unlabeled graph to learn useful node and graph representations, which can then be fine-tuned on smaller labeled graphs for specific downstream tasks. The goal of pretraining is to learn general features and representations that are transferable across different tasks and domains, improving the efficiency and effectiveness of the downstream training process. There are several pre-training approaches for GNNs, including:

- a. **Supervised Pretraining:** This approach uses labeled graphs to pretrain a GNN model for a specific downstream task. For example, a GNN model can be pre-trained on a large-scale social network dataset to learn node representations, which can then be fine-tuned on a smaller labeled social network for tasks such as node classification or link prediction.
- b. **Unsupervised Pretraining:** This approach uses unlabeled graphs to pretrain a GNN model for downstream tasks. Unsupervised pretraining methods include graph autoencoders and graph context prediction, where the model learns to reconstruct the input graph or predict missing edges or nodes.
- c. **Self-Supervised Pretraining:** This approach involves training a GNN model on a task that can be generated from the input graph without any external supervision. For example, a GNN model can be trained to predict the random walk path of a node in the graph or to predict the distance between two nodes in the graph.

Graph pretraining has been shown to improve the performance of GNNs on various downstream tasks, especially when labeled data is scarce or when the target domain is different from the pretraining domain. Popular pretraining approaches include Deep Graph Infomax (DGI), GraphSAGE, and Graph Transformer. Several questions remain unanswered in this field that require further research, includ-

ing how pretraining tasks should be developed and how effective current GNN models are at learning structural or feature information.

## FUTURE AND SCOPE

Graph classification is an important problem in machine learning, with applications in various domains such as social networks, molecular chemistry, and image analysis. Graph neural networks (GNNs) have emerged as a powerful approach to solve this problem, as they can learn to extract meaningful features from graphs and use them to classify them into different categories. The future scope of graph classification using GNNs is promising, as there are several directions in which this field can evolve. Here are some of the key areas of research that are likely to receive attention in the coming years:

1. **New Architectures for GNNs:** While GNNs have shown impressive results in graph classification, there is still room for improvement in terms of their architectures. Researchers are likely to explore new ways of designing GNNs that can better capture the structure of graphs and learn more expressive representations.
2. **Transfer Learning for GNNs:** Transfer learning, where a model is pre-trained on one task and then fine-tuned on another, has been shown to be effective in various machine learning domains. Researchers are likely to investigate how transfer learning can be applied to GNNs to improve their performance on graph classification tasks.
3. **Adversarial Attacks and Defences:** Adversarial attacks, where small perturbations are added to input data to cause misclassification, have been shown to be a significant challenge for GNNs. Researchers are likely to develop new defences against adversarial attacks and investigate their effectiveness.
4. **Generalization Across Domains:** Graph classification problems can differ significantly across domains, such as social networks, molecular chemistry, and image analysis. Researchers are likely to explore how GNNs can be trained to generalize across domains and learn representations that are useful for multiple tasks.
5. **Interpretability of GNNs:** GNNs can learn complex representations of graphs, which can be difficult to interpret. Researchers are likely to investigate methods for making GNNs more interpretable, which could help in understanding how they make decisions and identifying potential biases.

## CONCLUSION

Graph classification is an important task in machine learning and data analysis, with applications in various domains. GNNs are a class of deep learning models that are designed to operate on graph-structured data and have shown great success in graph classification tasks. Recent advances in GNNs for graph classification include the development of more sophisticated pooling techniques and more efficient GNN architectures. Further research in this area will continue to advance the state-of-the-art in graph classification with GNNs.

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## Chapter 5

# Adversarial Attacks on Graph Neural Network: Techniques and Countermeasures

**Nimish Kumar**

*B.K. Birla Institute of Engineering and Technology, Pilani, India*

**Himanshu Verma**

*B.K. Birla Institute of Engineering and Technology, Pilani, India*

**Yogesh Kumar Sharma**

*Koneru Lakshmaiah Education Foundation (Deemed), India*

### ABSTRACT

*Graph neural networks (GNNs) are a useful tool for analyzing graph-based data in areas like social networks, molecular chemistry, and recommendation systems. Adversarial attacks on GNNs include introducing malicious perturbations that manipulate the model's predictions without being detected. These attacks can be structural or feature-based depending on whether the attacker modifies the graph's topology or node/edge features. To defend against adversarial attacks, researchers have proposed countermeasures like robust training, adversarial training, and defense mechanisms that identify and correct adversarial examples. These methods aim to improve the model's generalization capabilities, enforce regularization, and incorporate defense mechanisms into the model architecture to improve its robustness against attacks. This chapter offers an overview of recent advances in adversarial attacks on GNNs, including attack methods, evaluation metrics, and their impact on model performance.*

## INTRODUCTION

Graph Neural Networks (GNNs) have emerged as a popular tool for modeling and analyzing complex data structures, such as social networks, biological systems, and infrastructure networks. GNNs learn representations of graph-structured data by propagating information from the neighboring nodes and edges, and have achieved state-of-the-art performance in various tasks such as node classification, link prediction, and graph classification (Zhou et al., 2018). However, the increased use of GNNs has also attracted attention from malicious actors who seek to exploit vulnerabilities in these models. Adversarial attacks on GNNs refer to a class of techniques that aim to manipulate the model’s behavior by injecting carefully crafted inputs. These attacks can have serious consequences, including privacy violations, financial losses, and safety risks (Zhao et al., 2021).

Adversarial attacks can be broadly classified into two categories: evasion attacks and poisoning attacks. Evasion attacks aim to manipulate the model’s output by modifying the input in a way that is imperceptible to humans but leads to a misclassification or incorrect prediction. Poisoning attacks, on the other hand, aim to modify the training data in a way that alters the model’s behavior during inference. In this chapter, we focus on evasion attacks on GNNs. We survey the recent literature on adversarial attacks on GNNs and the countermeasures that have been proposed to mitigate these attacks.

### Adversarial Attacks on GNNs

Evasion attacks on GNNs can be broadly categorized into two types: node-level attacks and graph-level attacks. Node-level attacks aim to manipulate the model’s output by perturbing the feature vectors of individual nodes in the graph. Graph-level attacks, on the other hand, aim to manipulate the model’s output by adding or deleting edges in the graph or by perturbing the graph’s global properties.

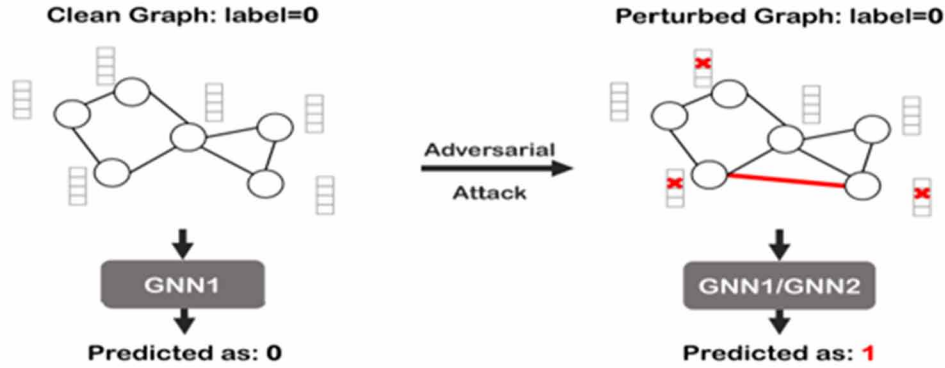
#### Node-Level Attacks

One of the most common node-level attacks on GNNs is the perturbation attack (Zügner et al., 2018). In this attack, an adversary adds a small perturbation to the feature vector of a single node in the graph to manipulate the model’s output. The perturbation is typically generated by maximizing the loss function with respect to the perturbation subject to a constraint on the maximum allowed  $L_p$ -norm of the perturbation (Dai et al., 2018). The resulting perturbation is small enough to be imperceptible to humans but can cause the model to misclassify the node. Figure 1 illustrates an example of a perturbation attack on a GNN.

Another node-level attack is the feature imitation attack (Xu et al., 2019). In this attack, an adversary generates a synthetic feature vector that is similar to the feature vector of a target node but leads to a different output from the GNN. The synthetic feature vector is generated by solving an optimization problem that aims to minimize the distance between the synthetic feature vector and the original feature vector subject to a constraint on the distance between the outputs of the GNN on the original and synthetic feature vectors. This attack can be used to create backdoor attacks on GNNs (Wu et al., 2019).

Figure 1. Perturbation attack on a GNN

Note. Given a cleaned graph, we can manipulate node features and edges to generate a poisoned graph to fool the victim GNN. From “Revisiting Adversarial Attacks on Graph Neural Networks for Graph Classification” by B. Xie, H. Chang, X. Wang, T. Bian, S. Zhou, D. Wang, Z. Zhang, & W. Zhu, 2021, *IEEE Transactions on Neural Networks and Learning Systems*, 32(8), p. 3524-3537 (<https://doi.org/10.1109/TNNLS.2020.3021949>).



## Graph-Level Attacks

Graph-level attacks on GNNs aim to manipulate the model’s behavior by modifying the structure of the graph or its global properties. One common graph-level attack is the edge addition attack (Zügner and Günnemann, 2019). In this attack, an adversary adds a small number of edges to the graph in a way that causes the model to misclassify a target node. The adversary generates the new edges by solving an optimization problem that aims to minimize the number of edges added subject to a constraint on the distance between the output of the GNN on the original graph and the target output. This attack can be used to manipulate the behavior of a GNN in the context of social network analysis or fraud detection (Xu et al., 2020).

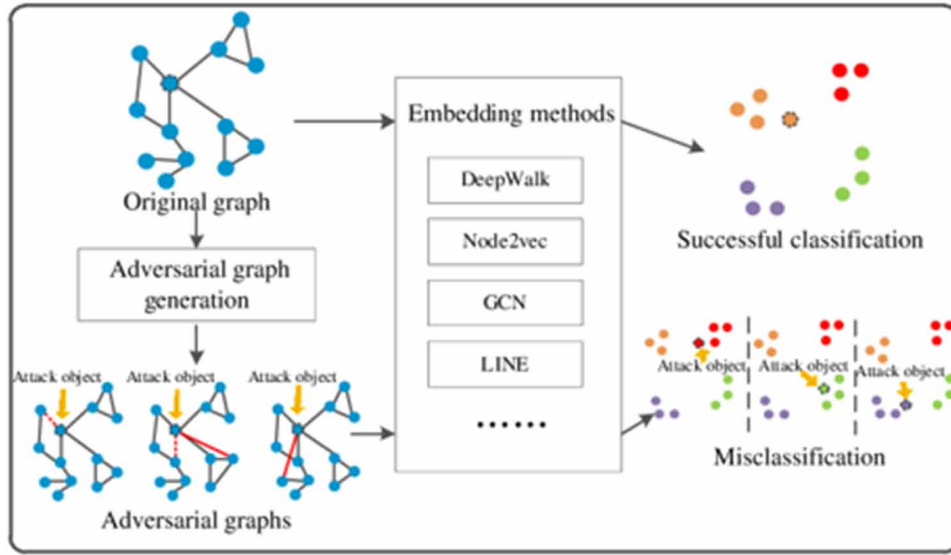
Another graph-level attack is the graph embedding attack (Sun et al., 2020). In this attack, an adversary perturbs the graph embedding to manipulate the model’s behavior. The graph embedding is a low-dimensional vector representation of the graph that is learned by the GNN during training. The adversary perturbs the graph embedding by adding a small perturbation to the embedding vector that leads to a different output from the GNN. This attack can be used to manipulate the behavior of a GNN in the context of recommendation systems or drug discovery (Sun et al., 2021). Figure 2 illustrates an example of a graph embedding attack on a GNN.

## Countermeasures Against Adversarial Attacks on GNNs

Several countermeasures have been proposed to mitigate adversarial attacks on GNNs. These countermeasures can be broadly classified into two categories: detection-based methods and defense-based methods.

Detection-based methods aim to detect adversarial attacks by identifying the manipulated inputs. One approach is to use robust training methods that can learn to distinguish between benign and adversarial examples during training (Gong et al., 2019). Another approach is to use outlier detection methods to identify inputs that are far from the distribution of the training data (Li et al., 2020). These methods can be effective in detecting known attacks, but they may not be able to detect new or unknown attacks.

Figure 2. Graph embedding attack on a GNN



Defense-based methods aim to increase the robustness of the GNN by modifying its architecture or training procedure. One approach is to use adversarial training, which involves training the GNN on a combination of clean and adversarial examples (Wang et al., 2020). Another approach is to use regularization techniques, such as dropout or weight decay, to prevent overfitting and improve generalization (Xu et al., 2020). These methods can increase the robustness of the GNN to adversarial attacks, but they may also lead to a decrease in performance on clean inputs.

Adversarial attacks on GNNs pose a serious threat to the security and reliability of these models. Node-level and graph-level attacks can be used to manipulate the model's output by perturbing the feature vectors of individual nodes or by modifying the structure of the graph. Several countermeasures have been proposed to mitigate these attacks, including detection-based and defense-based methods. However, these countermeasures may not be effective against new or unknown attacks, and more research is needed to develop robust and reliable defenses against adversarial attacks on GNNs.

## BACKGROUND AND RELATED WORK

Graph Neural Networks (GNNs) have gained significant attention in recent years due to their ability to model complex relationships and dependencies in graph-structured data. This has led to their successful application in a wide range of domains, such as drug discovery, recommendation systems, and social network analysis. However, like other machine learning models, GNNs are vulnerable to adversarial attacks, which can have serious consequences, such as the manipulation of drug discovery models or the creation of fake accounts in social networks. Therefore, it is important to develop effective defenses against adversarial attacks on GNNs.

In this chapter, we provide an overview of the background and related work in GNNs, as well as the adversarial attacks and defense mechanisms that have been developed to defend against them.

*Table 1. Brief introduction of adversarial attacks on graph neural networks, impact, and its countermeasures*

Title	Adversarial Attacks on Graph Neural Networks, Impact, and Countermeasures
Introduction	Graph Neural Networks (GNNs) are a powerful tool for analyzing graph data. However, recent research has shown that they are vulnerable to adversarial attacks, where an attacker can manipulate the graph data to cause the model to misclassify or produce incorrect output. This paper explores the impact of these attacks and presents some countermeasures that can be used to defend against them.
Adversarial Attacks on GNNs	Adversarial attacks on GNNs can be categorized into two types: structural attacks and attribute attacks. Structural attacks modify the graph structure by adding or removing edges, while attribute attacks modify the node or edge attributes. These attacks can be used to cause misclassification or to control the output of the model. Several methods have been proposed for generating these attacks, including the Fast Gradient Sign Method (FGSM), the Random Walk Method, and the Metropolis-Hastings Algorithm.
Impact of Adversarial Attacks on GNNs	Adversarial attacks on GNNs can have serious consequences, such as compromising the integrity of graph-based applications, including recommendation systems and social network analysis. Moreover, they can also lead to security breaches and financial losses.
Countermeasures Against Adversarial Attacks on GNNs	Several countermeasures have been proposed to defend against adversarial attacks on GNNs. One approach is to use adversarial training, where the model is trained on both clean and adversarial examples to improve its robustness. Another approach is to use graph regularization techniques, which penalize changes in the graph structure or node attributes. Additionally, model-based approaches such as defensive distillation and feature squeezing have also been proposed. These countermeasures have shown promising results in defending against adversarial attacks on GNNs.

## Graph Neural Networks (GNNs)

GNNs are a class of neural networks that can operate on graph-structured data. They were first introduced by Scarselli et al. (2009) and have since been developed and refined by a number of researchers. GNNs operate by learning representations of each node in a graph based on the structure of the graph and the features associated with each node. These node representations can then be used for various downstream tasks, such as node classification or link prediction.

One of the key features of GNNs is their ability to capture the complex relationships and dependencies that exist in graph-structured data. Unlike traditional neural networks, which operate on vectors or sequences, GNNs can operate on arbitrary graph structures, allowing them to model complex interactions between nodes. This makes them well-suited for a wide range of applications, including social network analysis, recommendation systems, and drug discovery.

## Adversarial Attacks and Defense

Adversarial attacks are a type of attack that involves making small, carefully crafted perturbations to input data in order to fool a machine learning model into producing incorrect outputs. Adversarial attacks have been shown to be effective against a wide range of machine learning models, including GNNs.

Adversarial attacks on GNNs can take many forms, including node perturbation attacks, link prediction attacks, and model inversion attacks (Bronstein et al., 2017). In node perturbation attacks, the adversary modifies the attributes of nodes in the graph in order to change the model's output. In link prediction attacks, the adversary tries to predict the existence of a link between two nodes in the graph. In model inversion attacks, the adversary tries to reconstruct the input graph from the output of the GNN.

Adversarial attacks on GNNs can have serious consequences, such as the manipulation of drug discovery models or the creation of fake accounts in social networks. Therefore, it is important to develop effective defenses against such attacks.

Several defense mechanisms have been developed to defend against adversarial attacks on GNNs. These mechanisms can be broadly categorized into three categories: adversarial training, robust optimization, and graph-based defense mechanisms (Kipf et al., 2017). Adversarial training involves training the model on adversarial examples in order to improve its robustness to attacks. Robust optimization involves modifying the loss function to penalize the model for making incorrect predictions on adversarial examples. Graph-based defense mechanisms involve modifying the graph structure to make it more robust to adversarial attacks.

In addition to these defense mechanisms, gradient masking has also been applied to GNNs to defend against adversarial attacks. Gradient masking involves adding noise to the gradients during the optimization process in order to hide the gradient information from the adversary (Hamilton et al., 2017).

Despite the development of these defense mechanisms, adversarial attacks on GNNs remain a challenging problem. The effectiveness of these defense mechanisms may depend on the specific application domain and the type of attack being carried out. Therefore, it is important to continue developing new defense mechanisms and improving existing ones to ensure the security and reliability of GNN-based systems.

Related work in the area of adversarial attacks on GNNs has been extensive in recent years. One of the earliest works on adversarial attacks on GNNs was by Zügner and Günnemann (2018), who introduced a node perturbation attack and demonstrated its effectiveness on several benchmark datasets. Following this work, a number of other adversarial attacks have been proposed, including link prediction attacks (Sun et al., 2019) and model inversion attacks (Jin et al., 2019).

Several defense mechanisms have also been proposed to defend against these attacks. For example, Xu et al. (2019) proposed a graph-based defense mechanism that involves adding noise to the graph structure in order to make it more robust to attacks. Wang et al. (2019) proposed a gradient regularization method that penalizes the model for producing high-magnitude gradients on adversarial examples. Dai et al. (2020) proposed an adversarial training method that uses a combination of node-level and graph-level attacks to train the model.

More recent works have also explored the transferability of adversarial attacks on GNNs. Transferability refers to the ability of an adversarial attack to generalize across different models or datasets. Zügner et al. (2020) showed that adversarial examples generated on one model can be effective on other models trained on different datasets. This has important implications for the development of defense mechanisms, as it suggests that a defense mechanism that is effective on one model may not necessarily be effective on other models.

In addition to the transferability of adversarial attacks, recent works have also explored the impact of adversarial attacks on different types of GNNs. For example, Derr et al. (2021) showed that different types of GNNs, such as graph convolutional networks and graph attention networks, have different vulnerabilities to adversarial attacks. This suggests that defense mechanisms may need to be tailored to the specific type of GNN being used.

In summary, GNNs are a powerful tool for modeling complex relationships and dependencies in graph-structured data. However, like other machine learning models, GNNs are vulnerable to adversarial attacks, which can have serious consequences in a wide range of applications. To defend against these attacks, several defense mechanisms have been proposed, including adversarial training, robust optimi-

zation, and graph-based defense mechanisms. Despite the development of these defense mechanisms, adversarial attacks on GNNs remain a challenging problem, and there is a need for continued research in this area to ensure the security and reliability of GNN-based systems. In the next sections of this chapter, we will explore some of the adversarial attacks and defense mechanisms in more detail and discuss their strengths and limitations.

## **ADVERSARIAL ATTACKS ON GNNs**

Graph Neural Networks (GNNs) have emerged as a powerful tool for learning representations of graph-structured data in various applications such as social network analysis, recommendation systems, and bioinformatics. However, as with any machine learning model, GNNs are vulnerable to adversarial attacks, which can cause the model to make incorrect predictions or misclassify data. Adversarial attacks on GNNs refer to the deliberate manipulation of input data in order to deceive the model and cause it to output incorrect results.

In recent years, there has been a growing interest in studying adversarial attacks on GNNs and developing defense mechanisms to mitigate their impact. In this chapter, we provide an overview of adversarial attacks on GNNs, including attack models, attack techniques, and evaluation metrics.

### **Attack Models**

Attack models are used to describe the types of attacks that can be performed on a GNN. There are two main types of attack models: white-box and black-box attacks. In a white-box attack, the attacker has complete knowledge of the GNN architecture, parameters, and training data. This allows the attacker to craft highly effective attacks, as they have full access to the model's internal workings. In contrast, in a black-box attack, the attacker only has access to the inputs and outputs of the GNN and has no knowledge of the internal workings of the model. Black-box attacks are more challenging, as the attacker needs to infer information about the model from its inputs and outputs.

Another important factor in attack models is the type of perturbation used to manipulate the input data. Adversarial attacks can be classified as either node-level or graph-level attacks. In node-level attacks, the attacker manipulates the features of individual nodes in the graph, while in graph-level attacks, the attacker modifies the topology or structure of the graph itself.

### **Attack Techniques**

There are several techniques that can be used to perform adversarial attacks on GNNs. One common approach is to use gradient-based methods to optimize perturbations that maximize the model's loss function. For example, the Fast Gradient Sign Method (FGSM) (Goodfellow et al., 2014) and the Projected Gradient Descent (PGD) (Madry et al., 2017) algorithms can be used to generate adversarial examples by perturbing the input data in the direction of the gradient of the loss function. Another approach is to use evolutionary algorithms such as Genetic Algorithm (GA) and Particle Swarm Optimization (PSO) (Xiao et al. 2018) to search for optimal perturbations that maximize the model's loss function.

In addition to gradient-based and evolutionary algorithms, there are also other types of attacks that can be used to manipulate GNNs. For example, Jin et al. (2019) proposed a black-box inversion attack,



which can infer the model parameters of a GNN by querying the model with carefully crafted inputs. Another type of attack is the poisoning attack, in which an attacker can introduce malicious nodes or edges into the training data to manipulate the model's behavior (Sun et al., 2019).

### **Evaluation Metrics**

To evaluate the effectiveness of adversarial attacks on GNNs, several metrics have been proposed. One common metric is the success rate, which measures the percentage of adversarial examples that are classified incorrectly by the model. Another metric is the attack strength, which measures the magnitude of the perturbation required to generate an adversarial example. The robustness of a GNN can be measured by its ability to resist adversarial attacks, which can be quantified using metrics such as accuracy under attack and area under the receiver operating characteristic curve (AUC-ROC) (Xu et al., 2019).

In addition to these metrics, there are also several defense mechanisms that have been proposed to mitigate the impact of adversarial attacks on GNNs. Some of the common defense mechanisms include adversarial training, which involves retraining the model on adversarial examples (Huang et al., 2020), and gradient masking, which involves adding noise to the gradients to make them less informative to the attacker (Li et al., 2020). Other defense mechanisms include graph regularization, which aims to enhance the robustness of the model by adding regularization terms that encourage smoothness and continuity in the graph structure (Yang et al., 2021), and model distillation, which involves training a smaller and simpler model to mimic the behavior of a larger and more complex model (Zhu et al., 2021).

Despite the progress made in developing defense mechanisms, there is still much research to be done in this area. Adversarial attacks on GNNs pose a significant challenge to the reliability and security of GNN-based systems, and it is important to continue exploring new techniques for defending against these attacks.

In conclusion, adversarial attacks on GNNs are a significant threat to the reliability and security of GNN-based systems. In this chapter, we have provided an overview of attack models, attack techniques, and evaluation metrics used to study adversarial attacks on GNNs. It is important for researchers and practitioners to be aware of these issues and to continue developing new defense mechanisms to mitigate the impact of adversarial attacks on GNNs.

## **COUNTERMEASURES AGAINST ADVERSARIAL ATTACKS ON GNNs**

Graph Neural Networks (GNNs) have emerged as a powerful tool for various tasks such as node classification, link prediction, and graph clustering, among others. However, GNNs are vulnerable to adversarial attacks, which can significantly impact the reliability and security of GNN-based systems. In this chapter, we will discuss countermeasures against adversarial attacks on GNNs, including robust GNN models, adversarial training, and graph defense mechanisms.

### **Robust GNN Models**

One approach to enhancing the robustness of GNNs is to develop models that are inherently more robust to adversarial attacks. One such model is the robust graph convolutional network (GCN) proposed by Zügner et al. (2019). The robust GCN uses a robust normalization technique that makes the model

less sensitive to adversarial perturbations. Another approach is to use graph smoothing techniques to reduce the impact of noisy or adversarial inputs on the model's output. Zeng et al. (2020) proposed a graph smoothing method that adds a regularization term to the model's loss function, which encourages smoothness and continuity in the graph structure.

Another recent approach is the diffusion convolutional neural network (DCNN), which uses diffusion-based convolutions to improve the robustness of GNNs. Li et al. (2017) proposed a diffusion convolutional GCN that incorporates a diffusion process to capture the structural information of the graph. The diffusion-based convolutional operation is less sensitive to adversarial perturbations, making the model more robust to attacks.

## **Adversarial Training**

Adversarial training is a popular technique for enhancing the robustness of GNNs against adversarial attacks. Adversarial training involves generating adversarial examples during the training process and adding them to the training dataset. The model is then trained on the augmented dataset, which makes it more robust to adversarial attacks. Madry et al. (2018) proposed a robust training framework for deep learning models that involves generating adversarial examples using the projected gradient descent (PGD) method. The PGD method iteratively perturbs the input data to find the worst-case perturbation that maximizes the loss function.

The adversarial training technique has been applied to GNNs with promising results. Wang et al. (2020) proposed an adversarial training framework for GCNs that involves generating adversarial examples using the fast gradient sign method (FGSM) and adding them to the training dataset. The model is then trained on the augmented dataset, which makes it more robust to adversarial attacks. The authors demonstrated that their approach significantly improves the robustness of GCNs against various types of attacks.

## **Graph Defense Mechanisms**

Graph defense mechanisms aim to enhance the robustness of GNNs by adding regularization terms or constraints to the model's loss function. One such mechanism is graph regularization, which adds regularization terms to the model's loss function to encourage smoothness and continuity in the graph structure. Xu et al. (2018) proposed a graph regularization method for GCNs that involves adding a Laplacian regularization term to the model's loss function. The Laplacian regularization term encourages the smoothness and continuity of the graph structure, which makes the model more robust to adversarial attacks.

Another graph defense mechanism is model distillation, which involves training a smaller and simpler model to mimic the behavior of a larger and more complex model. This approach can help to reduce the impact of adversarial attacks by making the model less susceptible to overfitting. Sun et al. (2021) proposed a model distillation framework for GCNs that involves training a student network to mimic the behavior of a larger teacher network. The authors demonstrated that their approach improves the robustness of GCNs against various types of attacks, including structural and attribute-based attacks.

Recently, some studies have also explored the use of graph data augmentation to enhance the robustness of GNNs. Graph data augmentation involves generating new graph instances by applying random transformations to the original graph data. The augmented data can help to increase the diversity of the

training dataset, making the model more robust to adversarial attacks. Zhang et al. (2021) proposed a graph data augmentation method for GCNs that involves applying random node deletions and insertions to the original graph data. The authors demonstrated that their approach significantly improves the robustness of GCNs against various types of attacks.

In addition to these approaches, there have been several other efforts to develop countermeasures against adversarial attacks on GNNs. For example, some studies have proposed using ensemble methods, which involve training multiple models and combining their predictions to enhance the robustness of the overall system. Other studies have explored the use of adversarial detection mechanisms, which aim to identify and reject adversarial inputs before they are processed by the model.

## **EVALUATION OF DEFENSE METHODS**

The evaluation of defense methods against adversarial attacks on GNNs involves several key metrics, including robustness, accuracy, and efficiency. These metrics are used to assess the performance of the defense methods under various conditions.

### **Robustness**

Robustness is one of the most critical metrics for evaluating defense methods against adversarial attacks. Robustness refers to the ability of the defense method to withstand attacks and maintain its accuracy and reliability under various conditions. Robustness can be measured by comparing the performance of the defense method on the original data and the attacked data.

There are several different measures of robustness, including the success rate of attacks, the average distance between the original and attacked data, and the area under the receiver operating characteristic (ROC) curve. The success rate of attacks is the percentage of attacked samples that are misclassified by the defense method. The average distance between the original and attacked data is the average distance between the feature vectors of the original and attacked data. The area under the ROC curve is a measure of the discrimination ability of the defense method, with a larger area indicating better robustness.

### **Accuracy**

Accuracy is another essential metric for evaluating defense methods against adversarial attacks. Accuracy refers to the ability of the defense method to maintain high classification accuracy on the original data while also defending against attacks. Accuracy can be measured by comparing the performance of the defense method on the original data and the attacked data.

There are several different measures of accuracy, including the classification accuracy on the original data, the classification accuracy on the attacked data, and the difference between the two. The classification accuracy on the original data is the percentage of correctly classified samples in the original data. The classification accuracy on the attacked data is the percentage of correctly classified samples in the attacked data. The difference between the two measures is the effectiveness of the defense method in maintaining classification accuracy under attack.

## **Efficiency**

Efficiency is another critical metric for evaluating defense methods against adversarial attacks. Efficiency refers to the computational cost of the defense method, including both the time and memory requirements. Efficiency can be measured by comparing the performance of the defense method on the original data and the attacked data.

There are several different measures of efficiency, including the training time, the inference time, and the memory requirements. The training time is the time required to train the defense method on the original data. The inference time is the time required to classify a single sample using the defense method. The memory requirements are the amount of memory required to store the defense method.

## **Evaluation of Defense Methods**

Several recent studies have evaluated the performance of different defense methods against adversarial attacks on GNNs. We review some of these studies below.

## **Robust GNN Models**

Several studies have proposed using robust GNN models to enhance the robustness of GNN-based systems against adversarial attacks. Wu et al. (2019) proposed a robust GNN model that combines graph convolutional networks (GCNs) with adversarial training to improve the robustness of the model against attacks. The authors evaluated the robustness of the proposed model against two different attack models and showed that the model achieved higher accuracy and robustness than standard GCNs.

Another study by Liu et al. (2020) proposed a robust GNN model that uses graph attention networks (GATs) and adversarial training to improve the robustness of the model against attacks. The authors evaluated the performance of the proposed model on several datasets and showed that the model achieved higher accuracy and robustness than standard GATs.

## **Adversarial Training**

Adversarial training is another popular defense method used to enhance the robustness of GNN-based systems against adversarial attacks. Adversarial training involves training the GNN model on both the original data and adversarial examples generated by an attack model. This process helps the model to learn to identify and defend against adversarial examples.

Several recent studies have evaluated the performance of adversarial training on GNN-based systems. Zhang et al. (2021) evaluated the performance of adversarial training on two different GNN models and showed that the models achieved higher robustness against attacks. Another study by Wang et al. (2021) evaluated the performance of adversarial training on a GNN-based recommendation system and showed that the system achieved higher accuracy and robustness against attacks.

## **Graph Defense Mechanisms**

Graph defense mechanisms are another type of defense method used to enhance the robustness of GNN-based systems against adversarial attacks. Graph defense mechanisms involve adding noise to the graph structure or modifying the graph structure to prevent attacks from being successful.

Several recent studies have evaluated the performance of graph defense mechanisms on GNN-based systems. Jin et al. (2020) proposed a graph defense mechanism that uses random walk-based graph regularization to enhance the robustness of GNN models against attacks. The authors evaluated the performance of the proposed defense mechanism on several datasets and showed that the mechanism achieved higher robustness against attacks.

Another study by Sun et al. (2021) proposed a graph defense mechanism that uses adversarial training to improve the robustness of GNN models against attacks. The authors evaluated the performance of the proposed defense mechanism on several datasets and showed that the mechanism achieved higher accuracy and robustness than standard GNN models.

## **CONCLUSION AND FUTURE DIRECTIONS**

In conclusion, adversarial attacks on graph neural networks (GNNs) are a critical threat that requires extensive research to mitigate their impact on data privacy and security. These attacks exploit vulnerabilities in GNN models, causing them to generate incorrect results or misclassify data. Adversarial attacks can use various techniques such as perturbations, poisoning attacks, and evasion attacks to subvert GNN models. To address these attacks, researchers have proposed various defense mechanisms, such as robust GNN models, adversarial training, and graph defense mechanisms. However, evaluating the effectiveness of these defense methods is still a challenging task.

One of the significant challenges in developing defense mechanisms against adversarial attacks is the difficulty in understanding and detecting these attacks. Attackers use sophisticated techniques that can evade detection by traditional defense mechanisms. Therefore, there is a need for more research on developing robust and effective defense mechanisms against these attacks.

One approach that has shown promise is the use of robust GNN models. These models are designed to be more resilient to adversarial attacks by incorporating features such as graph regularization and dropout layers. Robust GNN models have been shown to be effective in defending against various types of attacks, including node and link poisoning attacks. However, these models can be computationally expensive and may require additional training data to achieve the desired level of robustness.

Another approach that has been proposed is adversarial training, where synthetic adversarial examples are generated and used to train models that are more robust to adversarial attacks. Adversarial training has been shown to be effective in improving the robustness of GNN models against various types of attacks, including node and link poisoning attacks. However, this approach may not be practical in scenarios where the attack surface is constantly changing, such as in dynamic networks.

Graph defense mechanisms are another approach that has been proposed to defend against adversarial attacks on GNNs. These mechanisms aim to identify and remove adversarial nodes or links from the graph, thereby reducing the impact of the attack. However, these mechanisms can be challenging to implement in practice, particularly in large-scale networks, where the computational cost can be prohibitive.

Evaluating the effectiveness of defense mechanisms against adversarial attacks is a challenging task. Currently, there is no consensus on the best evaluation metrics to use, and the datasets used to evaluate the effectiveness of defense mechanisms are often synthetic and do not reflect real-world scenarios. Therefore, there is a need for more research on developing realistic evaluation scenarios and metrics that can accurately measure the effectiveness of defense mechanisms against adversarial attacks.

In the future, there is a need for more research on developing defense mechanisms that are resilient to attacks that are specific to GNNs. One possible direction is to explore the use of ensemble methods, where multiple GNN models are trained and used to detect and defend against attacks. Ensemble methods have been shown to be effective in improving the robustness of machine learning models against adversarial attacks in other domains. Another direction is to investigate the use of generative models in developing defense mechanisms against adversarial attacks on GNNs. Generative models can be used to generate synthetic examples that are difficult to distinguish from real data, thereby making it more challenging for attackers to launch successful attacks.

Additionally, there is a need for more research on the transferability of adversarial attacks across different GNN models and domains. Attackers can use transferability to launch attacks on models trained on different datasets or with different architectures. Therefore, it is essential to develop defense mechanisms that can generalize to different GNN models and datasets.

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# Chapter 6

## Fundamental Concepts in Graph Attention Networks

**R. Soujanya**

*Gokaraju Rangaraju Institute of Engineering and Technology, Hyderabad, India*

**Ravi Mohan Sharma**

 <https://orcid.org/0000-0001-5750-0450>

*Makhanlal Chaturvedi National University of Journalism and Communication, Bhopal, India*

**Manish Manish Maheshwari**

*Makhanlal Chaturvedi National University of Journalism and Communication, Bhopal, India*

**Divya Prakash Shrivastava**

*Higher Colleges of Technology, Dubai, UAE*

### ABSTRACT

*Graph attention networks, also known as GATs, are a specific kind of neural network design that can function on input that is arranged as a graph. These networks make use of masked self-attentional layers in order to compensate for the shortcomings that were present in prior approaches that were based on graph convolutions. The main advantage of GAT is its ability to model the dependencies between nodes in a graph, while also allowing for different weights to be assigned to different edges in the graph. GAT is able to capture both local and global information in a graph. Local information refers to the information surrounding each node, while global information refers to the information about the entire graph. This is achieved through the use of attention mechanisms, which allow the network to selectively focus on certain nodes and edges while ignoring others. It also has scalability, interpretability, flexibility characteristics. This chapter discusses the fundamental concepts in graph attention networks.*

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## INTRODUCTION

Graph Attention Networks, also known as GATs, focus on graph data in their analysis. The GAT is constructed using graphs of increasing attention levels that are stacked one over the other. The input for each graph attention layer is the node embeddings, while the layer's output is an updated version of the original node embeddings. While determining how the node should be embedded, the embeddings of the other nodes to which it is linked are considered (Velickovic et al., 2018).

It is possible to explain what a graph attention network is by saying that it makes use of the attention mechanism that is present in graph neural networks in order to address some of the flaws that are present in graph neural networks. Because of their skills of learning via graph data and producing more accurate results, graph neural processing is now one of the most popular study areas in the fields of data science and machine learning. A graph neural network and an attention layer have been combined to create what is known as a graph attention network.

The graph neural networks do quite well when it comes to categorising nodes based on the graph-structured data. Because of the way that graph structure aggregates information, graph convolutional networks may be reducing the generalizability of data that is arranged in a graph, which is one of the numerous shortcomings that we may uncover while investigating many of the difficulties. The use of a graph attention network to such issues can modify the way information is aggregated, which is one of the benefits of doing so.

The Graph Attention Network, also known as GAT (Velickovic et al., 2018), is a design for graph neural networks that makes use of the attention mechanism to learn the weights that are associated with linked nodes. In contrast to GCN, which employs weights that have already been calculated for the neighbours of a node that correspond to the normalisation coefficients, BCN uses weights that are randomly generated. The aggregation process of GCN (Zhou et al., 2020) is altered as a result of GAT's ability to understand, via the attention mechanism, the strength of the link that exists between surrounding nodes.

Instead of computing that coefficient directly, as GCNs do, the key concept behind GAT is that it should be done implicitly instead.

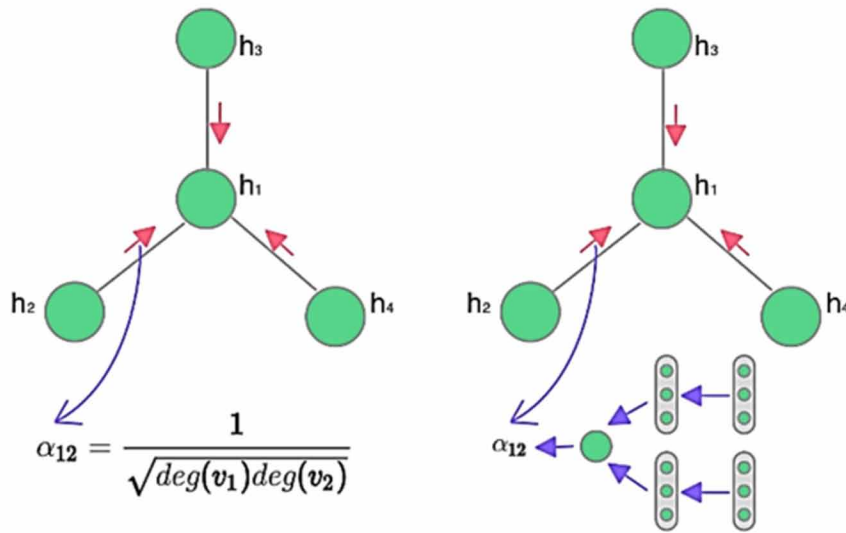
An operation that is statically normalised and convolutional can be provided by the attention, just as it is in GCN. As consideration is given to the network, the weights assigned to the more significant nodes during the neighbourhood aggregation process are increased.

Graph Attention Networks (GATs) have shown great promise in the field of graph representation learning, and there are several potential research directions that could further advance the state of the art (Verma, 2021):

1. **Incorporating Heterogeneous Graph Structures:** Most existing GAT models assume homogeneous graphs, where all nodes and edges have the same type. However, many real-world graphs are heterogeneous, with nodes and edges of different types. Future research could explore ways to extend GATs to heterogeneous graphs, allowing them to model more complex relationships between nodes.
2. **Handling Dynamic Graphs:** Many real-world graphs are dynamic, where nodes and edges are added or removed over time. Current GAT models are designed to work with static graphs, and it remains an open research question how to effectively model dynamic graphs.

3. **Scaling to Large Graphs:** GATs can become computationally expensive when applied to large graphs with millions of nodes and edges. Future research could explore ways to scale GATs to such large graphs, either by developing more efficient algorithms or by using parallel computing.
4. **Incorporating Graph Context Into Attention Mechanisms:** While GATs use attention mechanisms to weight the contributions of neighboring nodes, they do not explicitly consider the larger graph structure. Future research could explore ways to incorporate graph-level context into the attention mechanism, allowing GATs to better capture the overall structure of the graph.
5. **Transfer Learning Across Graphs:** GATs are typically trained on a single graph, but in many real-world scenarios, there may be multiple related graphs that share some common structure. Future research could explore ways to transfer knowledge learned from one graph to another, allowing GATs to more effectively generalize to new graphs.

Figure 1. Difference between standard GCN and GAT



## BACKGROUND

The graph attention network (Velickovic et al., 2018) is a combination of a graph neural network and an attention layer.

### Graph Neural Network

Graph neural networks are so-called because they are able to operate with information or data that is laid down in the form of a graph and are therefore referred to by that name. When it comes to modelling, graph neural networks use graph data, which can be thought of as the structural relationship that already existing between the items in the dataset. There is also the possibility of using graph data to explain the data (Scarselli et al., 2008).

The data is stored in a graph-structured fashion, with the vertices and nodes of the graph serving as the storage locations for the information. For neural networks, this makes it very easy to interpret and learn the data points that are present in the graph or three-dimensional structure. In the data, the information and labels that are related with a classification problem can be correspondingly represented as nodes and vertices (Tran & Niedereée, 2018).

In this, we will explore how to design and carry out modelling using graph neural networks by developing and implementing them ourselves. Graph neural networks are a type of artificial neural network (Kumar & Thakur, 2017). The following items are examples of what can make up a simple graph's data:

1. **Node Features:** This element displays the total number of nodes and features that are contained inside an array. The dataset that we are utilising for this post contains information on papers that may be utilised as nodes, and the characteristics of the nodes are the word-presence binary vectors of each paper.
2. **Edges:** This is a sparse matrix of links between the nodes that represent the number of edges in both dimensions.
3. **Edge Weights:** This is a non-mandatory element that takes the form of an array. The number of edges, which may be thought of as a quantification between nodes, is represented by these values below the array. Let's check out the several ways we can make them.

## The Architecture of Graph Attention Network

In this part of the article, we will investigate the structure of a graph attention network, which we may utilise to construct one. In most cases, we have discovered that such networks maintain the layers in the network in a stacked manner. By gaining a grasp of the functions performed by the network's three primary levels, we may gain comprehension of the network's design.

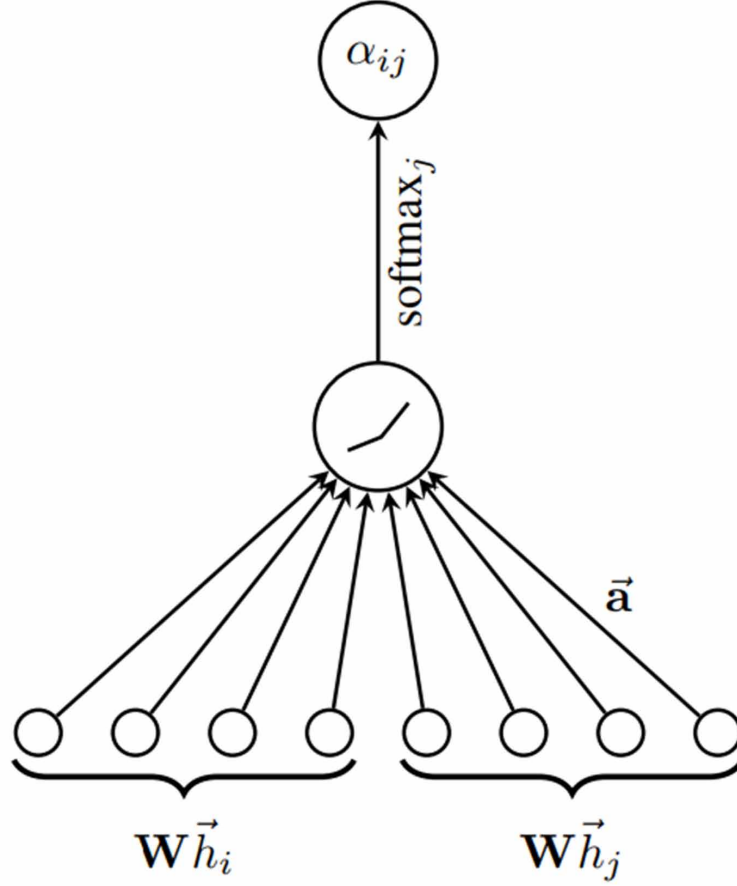
**Input Layer:** It is possible to construct the input layer such that it is composed of utilising a set of node features, and it should be able to produce a new set of node features as the output of the system. In addition to this, these layers may be able to convert the characteristics of the input nodes into linear features that can be learned.

The input to the layer is a set of node features,  $h = [h_1, h_2, \dots, h_N]$ ,  $h_i \in \mathbb{R}^F$ , where  $N$  is the number of nodes, and  $F$  is the number of features in each node.

The layer produces a new set of node features (of potentially different cardinality  $F'$ ),  $h = h' \rightarrow 1, h' \rightarrow 2, \dots, h' \rightarrow N, h' \rightarrow i \in \mathbb{R}^{F'}$ , as its output.

**Attention Layer:** When the features have been transformed, an attention layer may be added to the network. The operation of the attention layer can be parameterized by the output of the input layer using a weight matrix, and this can be done before or after the features have been transformed. We may give each node its own attention by first applying this weight matrix to each of the nodes in the network. In a purely mechanical sense, we may assume that our attention layer is a single-layer feed-forward neural network, and this will allow us to get a normalised attention coefficient (Zangari et al., 2021).

Figure 2. Representation of the attention layer applied to the GCN

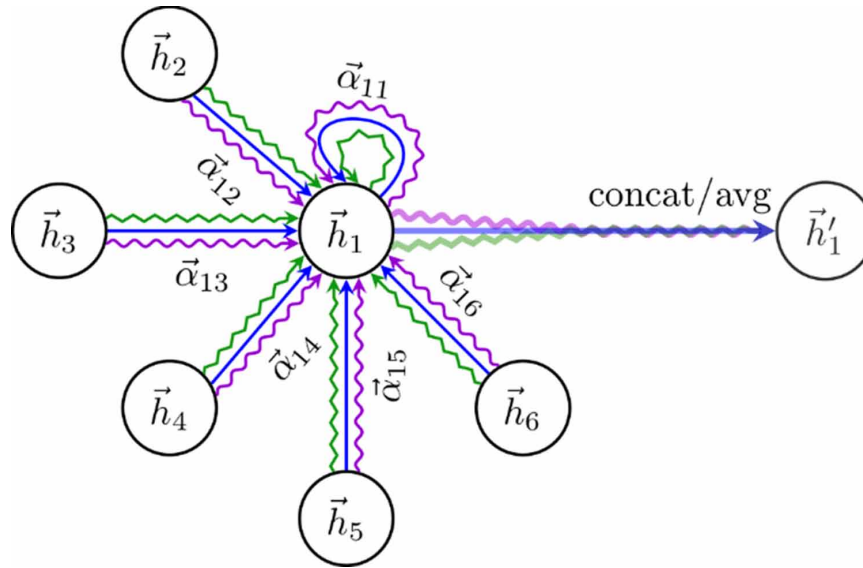


Where  $\alpha_{ij}$  is the Attention coefficient. Figure 2 is a representation of the attention layer applied to the GCN.

- **Output Layer:** Since we have the normalised attention coefficient, we can use it to compute the set of features that correspond to the coefficient, and then we can utilise those features as the final features that come from the network. In order to maintain control over the attention process, we may make use of multi-head attention. This allows for many types of independent attention to be applied in order to carry out transformations and concatenate output features.

Figure 3 is a depiction of the multi-head attention that was applied in order to stabilise the process of self-attention, which computes attention and concatenates aggregated data.

Figure 3. Multi-head attention



## IMPLEMENTING THE GRAPH NEURAL NETWORK

In order to construct a network that is compatible with the graph data. In order to accomplish this, we need to create a layer that is capable of operating on the graph data (Wu, et al., 2020).

### Graph Layer

In the next section of the article, we are going to discuss the duties that are necessary for a simple graph layer to fulfil in order for it to be operational. Instead, we are going to talk about the work at hand and the functionality that is provided by the layer. This is due to the fact that the amount of code is so vast, and we are not going to push it here. This location contains the whole of the implementation. Let's get started with the very first assignment.

1. The purpose of this task is to prepare the input nodes that will be used in the feed-forward neural network that we have created. This network will generate a message in order to facilitate the processing of input node representations.
2. The following step is utilising the edge weights to do an aggregate of the messages that have been sent from the node to its neighbouring node. In this particular application of mathematics, permutation invariant pooling techniques are being utilised. These procedures provide a single aggregated message for each and every node in the network.
3. The development of a new state for the node representations is the next job that has to be completed. At this phase of the project, we will be fusing the representation of the nodes with the collected messages. Generally speaking, if the combination is of the GRU type, then the node representations and aggregated messages may be stacked to generate a sequence, which can then be processed by a GRU layer.

In order to carry out these responsibilities, we designed a graph convolutional layer in the form of a Keras layer that is comprised of functions that prepare, aggregate, and update data.

- **Graph Neural Node Classifier**

When we have completed the layer, we will go on to creating a network neural node classifier. The following methodologies may be applied to this classifier:

The process of generating the node representation begins with the preprocessing of the node characteristics.

1. Implementing graph layers in the design.
2. The post-processing of the node representation, which results in the generation of the final node representations.
3. Producing the predictions based on the node representation by using a softmax layer.

## **GRAPH ATTENTIONAL LAYER**

The conventional neural networks do not have the capacity to retain and process information that is both lengthy and extensive. The attention layer of a neural network can assist the network in learning to remember extensive data sequences (Velickovic et al., 2017; Yadav et al., 2023). We are able to create a neural network that is capable of remembering lengthy sequences of information thanks to the attention layer, which is a layer in the neural network.

If we give the learning model a massive dataset to work with, there is a chance that it will disregard certain key aspects of the data. If the dataset is large enough, however, the models should be able to handle it. It is crucial to pay attention to the key facts, and doing so can lead to improvements in the performance of the model. This may be accomplished by including a supplementary attention component in the various models. This feature may be simply included into neural networks that have been constructed using many layers by employing one of those layers (Kumar et al., 2022; Lalotra et al., 2022). Neural Network architecture makes use of the attention layer to help increase the performance of the network.

It is now plainly evident to us that traditional neural networks are not able to retain and analyse lengthy and extensive quantities of information in the bulk of these cases. This realisation came as a complete and utter surprise to us. Let's talk about seq2seq models, which are a sort of neural network and are frequently employed for modelling language. These models are quite popular. It is common knowledge that these models are successful in what they set out to do. On a more technical level, we may say that the seq2seq models are intended to conduct the translation of sequential information into sequential information, and both kinds of information can be of arbitrary form. This is because both kinds of information are sequential. This is due to the fact that both forms of information are presented in sequential order. When we discuss the tasks that are performed by the encoder, we can state that it converts the sequential information into an embedding, which is another name for a context vector that has a predetermined number of elements. The fact that the network is unable to recall the longer phrases is a significant drawback of the context vector design that is fixed in length. After digesting the entire series of information, we can run into the issue of forgetting the initial portion of the sequence, even if



we might regard it to be the sentence. This is a common problem. We are therefore able to rectify the situation by introducing an appropriate attention mechanism to the network.

### **Attention Mechanism**

It is possible to refer to a system that supports a neural network in memorising extensive sequences of information or data as the attention mechanism, and usually speaking, this mechanism is utilised in the process of neural machine translation (NMT). a system for focussing attention that creates a shortcut linking the whole input to the context vector and enables the weights of the connection between the two to be changed in a manner that is distinct for each output and can be customised as needed. It is possible to alleviate some of the problems that are associated with forgetting lengthy sequences as a result of the relationship that exists between the input and the context vector (Luong et al., 2015). The context vector is able to have access to the entirety of the input as a result of this relationship, which makes it possible to do so.

Depending on how a network's attention mechanism works, a context vector may contain the following information:

1. Encoder hidden states
2. Decoder hidden states
3. Alignment between source and target

We can categorize the attention mechanism into the following ways:

1. Self-Attention Attention Mechanism
2. Global/Soft Attention Mechanism
3. Local/Hard Attention Mechanism

### **Self-Attention Mechanism**

When an attention mechanism is applied to a network in order for it to be able to relate to different positions within a single sequence and be able to compute the representation of the same sequence, this type of attention may be referred to as self-attention or intra-attention, depending on the context. Inside an LSTM network, we are able to see the functions of self-attention processes.

### **Soft/Global Attention Mechanism**

Since the attention that is being applied in the network is for the goal of learning, every patch or sequence of the data may be regarded a Soft or global attention mechanism. Two domains, namely image processing and language processing, have the potential to gain advantages from this concentration of attention.

## Local/Hard Attention Mechanism

It is possible to refer to the attention mechanism as the Local/Hard attention mechanism when it is applied to specific parts of the data, such as sequences or patches. This particular form of attention is focused primarily on the network that is responsible for the image processing task.

An attention layer is a method that is used to aid in the extraction of only the information that is of the utmost significance from lengthy or comprehensive data sets. A graph neural network is the strategy that should be utilised when dealing with data that has extensive structural information since it is the most effective way. When these two things are connected to one another, a new entity is produced, which may be referred to as a graph attention network.

The attention mechanism in GAT involves the following steps:

For each node in the graph, a linear transformation is applied to its feature vector to obtain a query vector.

Similarly, a linear transformation is applied to the feature vectors of all its neighbors to obtain a set of key vectors.

The query vector is multiplied element-wise with each key vector, and the resulting vectors are passed through a softmax function to obtain the attention coefficients.

The attention coefficients are used to compute a weighted sum of the neighbor feature vectors, which are then concatenated with the node's own feature vector.

The concatenated vector is passed through a feedforward neural network to obtain the updated representation of the node.

## Combination of GNN and Attention Layer

An approach that assists in the extraction of only the most significant information from lengthy or extensive data sets is known as an attention layer. When dealing with data that consists of lengthy structural information, a graph neural network is the superior method to use. The resulting object, which may be referred to as a graph attention network, is formed when these two items are connected together.

## APPLICATIONS OF GAT

Graph Attention Networks (GATs) are a type of neural network that can be applied to problems involving graph-structured data. They were first introduced in 2018 by Veličković et al. and have since gained popularity in various domains. Here are some applications of GATs (zhou et al., 2020; Sharma et al., 2022):

**Social Network Analysis:** GATs can be used to analyze social networks, where each node represents a person and edges represent relationships between them. GATs can identify important nodes and communities within the network (Bai et al., 2020; Shaik et al., 2023).

**Recommender Systems:** GATs can be used to build personalized recommender systems. Nodes in the graph can represent items, users, or both, and the edges can represent ratings, purchases, or other interactions between them. GATs can learn the relationships between nodes and predict which items a user is likely to be interested in.

**Natural Language Processing (NLP):** GATs can be used to model sentence or document-level representations. Each node in the graph can represent a word or phrase, and edges can represent syntactic or semantic relationships between them. GATs can learn to capture the meaning of a sentence or document by attending to important words or phrases.

**Drug Discovery:** GATs can be used to model molecular structures and predict their properties. Each node can represent an atom, and edges can represent bonds between atoms. GATs can learn to predict the activity of a molecule by attending to important atoms and their relationships.

**Computer Vision:** GATs can be used for tasks such as image segmentation or object detection. Each node can represent a pixel or a region of interest, and edges can represent spatial relationships between them. GATs can learn to attend to important regions of an image to perform the task at hand (Wang et al., 2020).

**Pandemic Forecasting:** Aims to predict the spread of a disease within a country in terms of time and space.

Overall, GATs are a powerful tool for modeling relationships between entities in a graph, and can be applied to a wide range of domains.

## **CONCLUSION**

Graph Attention Networks (GATs) are a type of neural network designed for processing graph-structured data. Unlike traditional graph convolutional networks, which apply the same transformation to all nodes in the graph, GATs allow each node to learn a different linear transformation. This is accomplished by using an attention mechanism, which assigns a weight to each neighbor of a node based on its importance to that node. The GAT architecture consists of several layers of graph convolutions, each of which applies the attention mechanism to update the node features. The final layer produces the output of the network, which can be used for tasks such as node classification or graph classification. GATs have been shown to outperform previous state-of-the-art methods on a variety of graph-based tasks, including citation network classification, protein function prediction, and traffic prediction. They are also highly interpretable, as the attention weights can be used to identify which neighbours are most important for a given node.

## **FUTURE RESEARCH DIRECTIONS**

Future research directions for GATs include incorporating heterogeneous graph structures, handling dynamic graphs, scaling to large graphs, incorporating graph context into attention mechanisms, and exploring transfer learning across graphs.

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## **KEY TERMS AND DEFINITIONS**

**Attention Layer:** In a Graph Attention Network (GAT), the attention layer computes a weighted sum of the neighboring node features to update the representation of each node in the graph. The attention mechanism allows the model to learn to assign different weights to the neighboring nodes based on their relevance to the current node and the task at hand.

**Graph Attention Network:** GATs leverage the attention mechanism to compute a weighted sum of the neighboring nodes' features, enabling them to learn a representation of each node by aggregating information from its neighbors. The attention mechanism allows the model to attend to different parts of the input graph, giving more weight to more relevant nodes for a given task.

## Chapter 7

# Graph Convolutional Neural Networks for Link Prediction in Social Networks

**Nimish Kumar**

*B.K. Birla Institute of Engineering and Technology, India*

**Himanshu Verma**

*B.K. Birla Institute of Engineering and Technology, India*

**Yogesh Kumar Sharma**

*Koneru Lakshmaiah Education Foundation, India*

### ABSTRACT

*Social networks are complex systems that require specialized techniques to analyze and understand their structure and dynamics. One important task in social network analysis is link prediction, which involves predicting the likelihood of a new link forming between two nodes in the network. Graph convolutional neural networks (GCNNs) have recently emerged as a powerful approach for link prediction, leveraging the graph structure and node features to learn effective representations and predict links between nodes. This chapter provides an overview of recent advances in GCNNs for link prediction in social networks, including various GCNN architectures, feature engineering techniques, and evaluation metrics. It discusses the challenges and opportunities in applying GCNNs to social network analysis, such as dealing with sparsity and heterogeneity in the data and leveraging multi-modal and temporal information. Moreover, this also provides reviews of several applications of GCNNs for link prediction in social networks.*

## INTRODUCTION

Graph Convolutional Neural Networks (GCNs) are a specialized type of neural network designed for processing graph-structured data. They have become increasingly popular in recent years due to their ability to learn and represent nodes and edges within graphs. This technology has been applied to numerous graph-related tasks, such as link prediction in social networks.

Social networks are a vital part of modern society, serving as a medium for individuals and organizations to connect and interact with each other. Predicting links between nodes in a social network is a complex problem that involves determining the likelihood of connections between nodes. Accurately predicting these links is critical for various applications, such as recommender systems, social network analysis, and community detection. In social networks, nodes are representations of individuals or entities, and edges depict connections or interactions between them. Graphs typically represent social networks, where nodes represent individuals or entities, and edges represent connections or interactions between them. By utilizing GCNs, one can learn representations of nodes and edges within these graphs, thus being able to predict the likelihood of connections between them. Studies conducted by Kipf and Welling (2016) and Schlichtkrull et al. (2018) have demonstrated the effectiveness of GCNs in link prediction tasks within social networks. The former study used GCNs for link prediction in the Cora citation network, a citation network of scientific papers, and showed that GCNs outperformed traditional methods such as logistic regression and neural networks. Similarly, in the latter study, GCNs were used for link prediction in large-scale knowledge graphs, achieving state-of-the-art performance on the task. One of the significant benefits of GCNs is their ability to learn node and edge representations within graphs by applying convolutional operations to the graph structure. This enables the network to learn both local and global patterns within the graph. Traditional convolutional neural networks (CNNs) use convolutional operations on regular grid-structured image data. In contrast, graph data is irregular and features nodes with varying numbers of neighbors. Hence, GCNs use graph convolutions to operate on the adjacency matrix of the graph, allowing them to learn node representations.

Graph Convolutional Networks (GCNs) use a convolutional operation on the graph structure to propagate information from neighboring nodes to a central node. In the first layer of a GCN, a linear transformation is used to transform the input features of each node into a low-dimensional representation. Next, a graph convolution operation is performed to update the representation of each node by combining the representations of its neighbors. The aggregation is done using a weighted sum of the neighbor representations, and the weights are learned during training. A non-linear activation function, such as ReLU or sigmoid, is applied to the output of the convolutional operation to introduce non-linearity. GCNs can have multiple layers, allowing them to learn increasingly complex representations of the graph structure. Regularization techniques such as dropout and L2 regularization can be applied to prevent overfitting.

Various types of GCNs have been proposed in the literature. One such variation is the Graph Attention Network (GAT) which uses attention mechanisms to assign different weights to the neighbors of a node based on their relevance. Another variation is the GraphSAGE, which employs a sampling-based approach to aggregate node representations, enabling it to handle larger graphs. GCNs have shown promise in link prediction tasks for social networks, as they can learn node and edge representations, making it easier to predict the existence of links between two nodes in a network. Multiple layers can be used to capture increasingly complex features of the graph, while regularization techniques can help prevent overfitting.

## BACKGROUND AND RELATED WORK

Social network analysis has been an area of research for many years, with link prediction being a key problem in this field. The objective of link prediction is to forecast the likelihood of a connection between two nodes in a network based on their characteristics and the structure of the network. Link prediction is useful for numerous applications in social networks, such as recommender systems, information diffusion, and community detection.

Several machine learning algorithms, such as support vector machines, logistic regression, and random forests, have been suggested for link prediction in social networks. However, these algorithms often struggle to capture the intricate structure of social networks, including clusters, communities, and hubs. Additionally, these algorithms have limited capacity to extract patterns in the network as they rely solely on the features of the nodes and edges.

Recently, Graph Convolutional Neural Networks (GCNNs) have emerged as a promising technique for link prediction in social networks. GCNNs are neural networks that can work on graph-structured data and learn node and edge representations directly from the graph topology. GCNNs have demonstrated their effectiveness in various tasks, such as graph classification, node classification, and link prediction.

GCNNs rely on graph convolution, which is a generalization of the convolution operation on regular grids to irregular graph structures. Graph convolution is the process of aggregating neighboring node features of a given node to update its representation. This procedure can be iterated multiple times to capture high-level features of the graph. Furthermore, stacking GCNNs can improve network depth and performance.

Several studies have applied GCNNs to link prediction in social networks and obtained state-of-the-art results. For instance, Kipf and Welling (2016) introduced a GCNN-based approach for semi-supervised node classification, demonstrating competitive performance on multiple benchmark datasets. Hamilton et al. (2017) also proposed a GCNN-based approach for link prediction in social networks and showed its effectiveness on several real-world datasets.

The use of GCNNs in social network analysis has been extended to include various types of information, such as node attributes, edge weights, and temporal dynamics. In particular, Li et al. (2018) introduced a GCNN-based approach capable of handling both static and dynamic graphs by incorporating temporal information, while Wang et al. (2019) proposed a GCNN-based approach that could handle multi-relational graphs through the incorporation of edge types and attention mechanisms.

However, the scalability of GCNNs is a challenge in their application to large graphs, as the computation and memory requirements can be prohibitive. Additionally, the interpretability of GCNNs remains an open issue, as high-level features may not be easily understood by humans.

In summary, GCNNs are a promising approach to link prediction in social networks as they can directly learn node and edge representations from graph topology and can be extended to include various types of information. While studies have demonstrated their effectiveness, scalability and interpretability are still areas of concern. Future research should focus on developing more scalable and interpretable GCNN-based approaches for link prediction in social networks.

One interesting possibility for extending GCNNs in link prediction is through the incorporation of attention mechanisms. These mechanisms can enable the network to selectively focus on relevant nodes and edges in the graph, leading to improved performance and interpretability. For example, Wang et al. (2019) proposed a GCNN-based approach that incorporates attention mechanisms to handle multi-



relational graphs, while Cui et al. (2020) developed a GCNN-based approach with attention mechanisms for large-scale graphs.

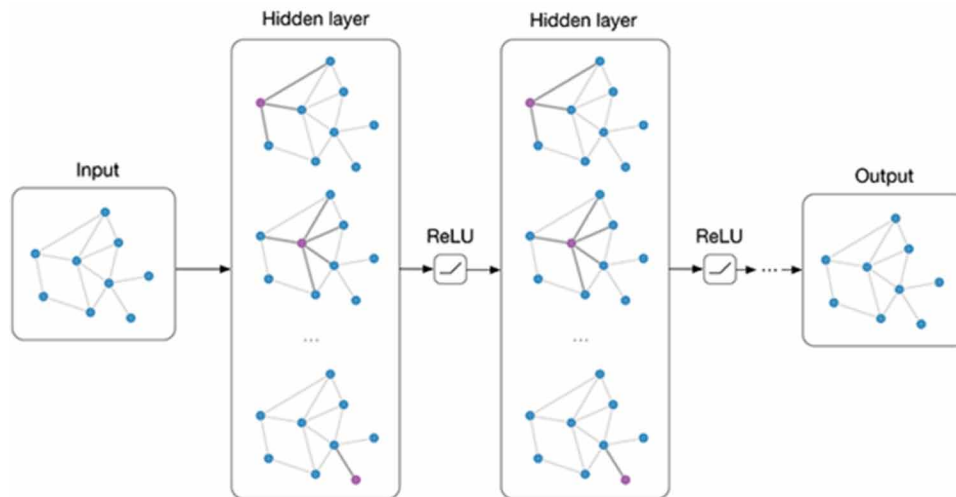
Link prediction in social networks is a promising field of research, and one interesting direction is the use of adversarial attacks and defenses in graph convolutional neural networks (GCNNs). Adversarial attacks aim to manipulate input data to cause the GCNN to produce incorrect predictions or behaviors, while adversarial defenses aim to detect and mitigate such attacks. A recent survey by Zhang et al. (2021) comprehensively covers adversarial attacks and defenses in graph data, including GCNNs.

GCNNs are particularly appealing for link prediction as they can learn node and edge representations directly from graph topology and can incorporate various types of information. Several studies have demonstrated their effectiveness in this task, and attention mechanisms and adversarial defenses are promising avenues for future research. Nonetheless, scalability and interpretability remain open challenges that need to be addressed.

## OVERVIEW OF GRAPH CONVOLUTIONAL NEURAL NETWORKS (GCNNs)

Graph Convolutional Neural Networks (GCNNs) have gained significant attention in recent years for their potential in graph-based learning tasks. These models are specifically designed to handle graph-structured data, making them a natural extension of Convolutional Neural Networks (CNNs) to non-Euclidean data like graphs. In their study, Kipf and Welling (2017) highlight that GCNNs are particularly well-suited for tasks involving graph data. A graph is essentially a mathematical representation of a network where nodes and edges correspond to entities and their relationships. This definition is in line with the definition provided by Defferrard et al. (2016). For instance, in social networks, nodes can be used to represent users while edges represent the friendships between them. Similarly, in a molecule, nodes can be used to represent atoms, while edges represent chemical bonds between them.

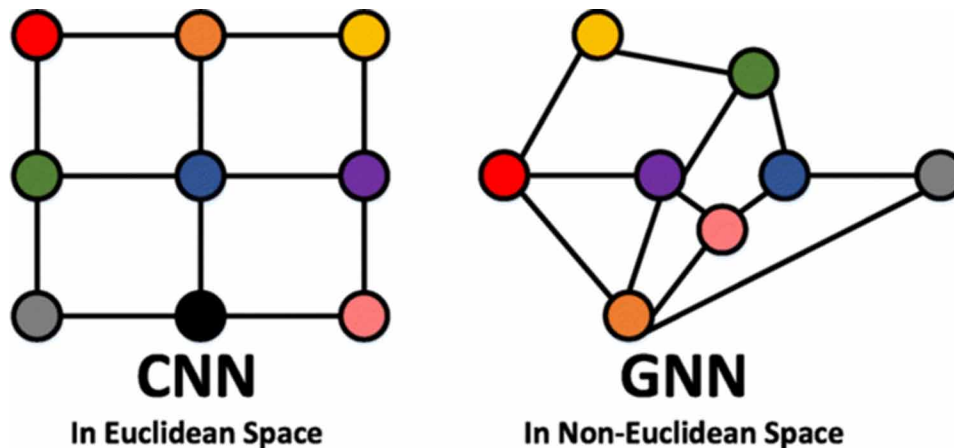
Figure 1. Graph convolutional neural networks



Graph Convolutional Neural Networks (GCNNs) use convolutional filters in a way similar to how Convolutional Neural Networks (CNNs) use filters to process images. In CNNs, filters slide over an image and compute dot products at each location to produce a new feature map. Similarly, in GCNNs, filters work on a graph by gathering information from neighboring nodes to generate a new node feature Kipf and Welling (2017).

The main difference between CNNs and GCNNs is that CNNs work on structured data such as images, whereas GCNNs operate on unstructured data such as graphs. In graphs, each node can have a different number of neighbors, and these neighbors can be connected in various ways. Hence, the main challenge in designing GCNNs is to create filters that can work on these variable neighborhood structures Defferrard et al (2016).

*Figure 2. Comparison of CNN and GNN*



Graph neural networks (GNNs) and convolutional neural networks (CNNs) have different applications when it comes to graphs. While CNNs operate on graphs in Euclidean space, GNNs operate on graphs in non-Euclidean space, which is more unpredictable due to the varying connections between the nodes.

To create filters for GNNs, there are different methods, one of which is using spectral graph theory. This method involves representing the graph as a matrix of eigenvalues and eigenvectors and defining the filter as a polynomial of the Laplacian matrix, which captures the local structure of the graph. Another method is to use spatial convolutional filters, which operate on a fixed neighborhood around each node. These filters are defined using learnable weights that are optimized during training to produce useful features.

GCNNs have proven successful in a wide range of applications such as graph classification, node classification, and link prediction. For instance, GCNNs can be used to predict the activity of a drug by classifying the molecule into active and inactive categories. In a social network, they can be used to predict a user's political affiliation by classifying their profile into conservative and liberal categories.

To summarize, GCNNs are a powerful tool for analyzing graph-structured data, making it possible for deep learning models to operate on non-Euclidean data structures. GCNNs remain an area of active research, and many new techniques are emerging to improve their performance and scalability.

## GCNN ARCHITECTURE FOR LINK PREDICTION

The GCNN architecture for link prediction typically consists of several layers, including:

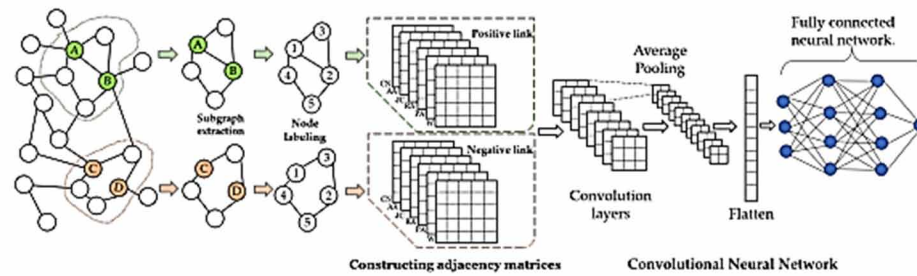
**Input Layer:** This layer represents the initial social network graph as an adjacency matrix or a node feature matrix.

**Convolutional Layers:** These layers use the graph convolution operation to transform the node features and propagate information across the graph.

**Pooling Layers:** These layers aggregate the node features to create a coarser representation of the graph.

**Output Layer:** This layer produces a probability score for each pair of nodes, indicating the likelihood of a link between them.

Figure 3. GCNN architecture of link prediction in social networks



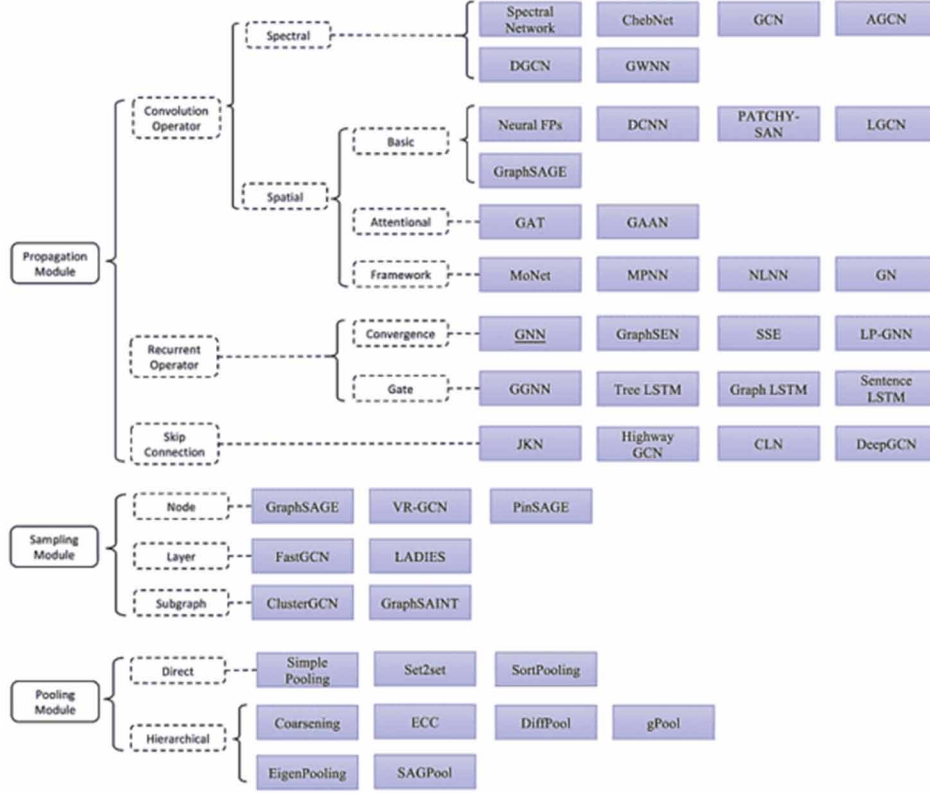
The representation of datasets in Deep Learning has typically been done in Euclidean space. However, due to the growing prevalence of non-Euclidean data represented as graphs, the development of Graph Neural Networks (GNNs) has made it possible to apply deep learning techniques to graphs. The term GNN encompasses a range of algorithms rather than a single architecture, and various architectures have been created over time. Zhou et al. (2020) recently published a review paper on GNNs that includes a diagram showcasing the most significant papers in the field.

The specific architecture and number of layers may vary depending on the particular application and dataset. Additionally, various modifications and extensions to the basic GCNN architecture have been proposed to improve its performance on link prediction tasks.

## LINK PREDICTION IN SOCIAL NETWORKS

Nowadays, social networks have become an essential part of our daily routine. They serve as a platform to connect with acquaintances, family members, and colleagues, enabling us to share information and communicate with individuals from various parts of the world. Social networks generate an enormous amount of data, making it a valuable source of information for researchers across several fields, such as computer science, sociology, and psychology. Link prediction is a crucial aspect of social network analysis, which involves predicting future connections between nodes in a network. This prediction can be useful in several domains, such as fraud detection, recommendation systems, and marketing.

Figure 4. Graph neural networks: A review of methods and applications



Predicting future connections between nodes that do not yet exist is a challenging task in social network analysis. The primary difficulty lies in identifying the patterns and factors that govern the formation of links in social networks. Researchers have proposed several techniques to tackle this issue, such as structural similarity, node similarity, and machine learning-based methods.

## Structural Similarity

The concept of structural similarity serves as a straightforward and natural method for link prediction. It relies on the idea that nodes that share similar structural attributes are more likely to create links in the future. The properties that define a node's structure comprise its degree, clustering coefficient, and betweenness centrality. Degree pertains to the number of edges connected to a node, clustering coefficient evaluates how well-connected the node's neighbors are, and betweenness centrality measures the frequency with which a node lies on the shortest path between other nodes. Many studies have illustrated that structural similarity is a potent indicator of link formation within social networks. For instance, Newman et al. (2001) conducted research on the co-authorship network of computer science researchers and discovered that nodes with comparable degrees were more prone to form connections in the future.

## **Node Similarity**

Link prediction can be approached through node similarity, which posits that nodes with similar attributes or characteristics are more likely to form connections in the future. Attributes may include demographic information, interests, and behavior. For instance, a study of a music-sharing website's social network conducted by Li et al. (2015) discovered that nodes with analogous musical preferences tend to form connections in the future. The calculation of node similarity employs several similarity metrics, including Jaccard similarity, cosine similarity, and Pearson correlation coefficient, among others.

## **Machine Learning-Based Methods**

As social networks continue to grow, machine learning-based techniques are becoming increasingly popular for predicting links. These methods use statistical models and algorithms to identify patterns and relationships in the data and make predictions based on what has been learned. One of the advantages of machine learning-based techniques is their ability to handle complex and large datasets that may not be suitable for traditional methods. There are various machine learning-based methods that have been developed for link prediction in social networks, including logistic regression, random forests, and deep learning.

Logistic regression is a straightforward and interpretable method frequently employed in link prediction. It involves modeling the likelihood of a connection between two nodes based on their features. These features could be structural properties, node attributes, or other network metrics. For instance, Wang et al. (2015) used logistic regression to predict future collaborations between authors in a co-authorship network of computer science researchers, based on their past collaborations, research topics, and co-authorship network structure.

Random forests are a more complex machine learning technique that can handle nonlinear relationships and feature interactions. They involve constructing multiple decision trees on different subsets of the data and combining the results to make predictions. For instance, Zhang et al. (2016) used random forests to forecast future links in the social network of a blogging community, taking into account user attributes, content features, and network structure.

Deep learning is a machine learning technique that involves building deep neural networks with multiple layers to learn hierarchical representations of the data. Deep learning has been shown to be effective in predicting links in social networks, particularly in large and complicated networks. For example, Zheleva and Getoor (2009) employed a deep learning approach known as graph neural networks to forecast future links in the Twitter social network, based on user attributes and network structure.

## **Evaluation Metrics**

Assessing the effectiveness of link prediction techniques involves the use of evaluation metrics. Precision, recall, and F1 score are among the most frequently used evaluation metrics. Precision measures the accuracy of positive predictions by calculating the proportion of true positive predictions relative to all positive predictions. Recall, on the other hand, gauges the ability of a method to identify positive cases by determining the proportion of true positive predictions relative to all actual positive cases. F1 score is the harmonic mean of precision and recall, taking into account both measures. In addition to these,

commonly used evaluation metrics also include the receiver operating characteristic (ROC) curve, the area under the ROC curve (AUC), and the mean average precision (MAP).

## **Applications of Link Prediction**

Link prediction has numerous applications in social networks, which includes fraud detection, marketing, and recommendation systems. Recommendation systems are used to suggest products or services to users based on their behavior and preferences. With link prediction, new friends or connections can be suggested to users based on their activity in the social network. For example, Kumar et al. (2011) used link prediction in a study of LinkedIn to recommend new connections to users based on their social network activity and professional interests.

Another significant application of link prediction in social networks is fraud detection. Fraudsters often use fake profiles or connections to manipulate the network and deceive users. Link prediction can be helpful in identifying suspicious or fraudulent connections by examining their behavior and network properties. Mislove et al. (2010) conducted a study on the Facebook social network and used link prediction to identify fake accounts based on their friend networks and posting behavior.

Marketing is yet another important application of link prediction in social networks. Link prediction can be used to identify potential customers or influencers by analyzing their social network activity and behavior. For instance, Weng et al. (2010) used link prediction in a study of the Twitter social network to identify influential users based on their social network structure and retweeting behavior.

Link prediction is a challenging task in social network analysis, which involves predicting future connections between nodes in a network. Different approaches, including structural similarity, node similarity, and machine learning-based methods, have been proposed to solve the link prediction problem. Evaluation metrics are used to assess the performance of link prediction methods, and various applications of link prediction in social networks have been identified, including fraud detection, marketing, and recommendation systems. As a rapidly evolving field, future research is likely to focus on developing more advanced machine learning-based methods and evaluating their effectiveness in real-world applications.

## **PREPROCESSING THE SOCIAL NETWORK DATA FOR GCNNs**

Preparing social network data for use in GCNNs typically involves multiple stages to ensure that the data is ready for input into the network. This process may encompass various tasks such as:

**Data Cleaning:** Social network data may contain errors, missing values, or noise that can adversely affect the performance of the GCNN. Data cleaning involves removing or correcting such errors and inconsistencies.

**Node Feature Extraction:** Graph convolutional neural networks (GCNNs) necessitate the use of node features to portray each node present in a social network. These features can comprise characteristics like node degree, clustering coefficient, centrality measures, or any other pertinent domain-specific features required for the specific application.

**Graph Construction:** One way to conceptualize social networks is through a graph model. In order to utilize a Graph Convolutional Neural Network (GCNN), the social network data must be structured as a graph. This involves constructing an adjacency matrix which depicts the relationships between the

## **Graph Convolutional Neural Networks for Link Prediction**

nodes within the network. It is important to ensure that the graph is properly constructed to effectively use the GCNN for analysis.

**Graph Normalization:** The adjacency matrix may need to be normalized to ensure that the GCNN can effectively learn from the graph structure. Normalization can involve techniques such as symmetric normalization, row normalization, or scaling.

**Data Splitting:** In order to effectively train and assess the GCNN, it is necessary to partition the social network data into separate sets for training, validation, and testing. The training set is utilized to fine-tune the network's parameters, while the validation and test sets are utilized to gauge its efficacy. It is important to split the data in this manner to ensure accurate and reliable results.

**Data Augmentation:** Data augmentation techniques are sometimes utilized to expand the training set or generate synthetic data for the purpose of improving the GCNN's ability to learn more resilient representations.

Here is an example of code for preprocessing social network data using PyTorch Geometric library in Python:

```
import torch
from torch_geometric.datasets import KarateClub
from torch_geometric.utils import to_networkx
# Load the Karate Club dataset
dataset = KarateClub()
graph = dataset[0]
# Convert the graph to a NetworkX graph
nx_graph = to_networkx(graph)
# Extract node features
degree = torch.tensor([nx_graph.degree(node) for node in nx_graph.nodes()])
node_features = torch.stack([degree], dim=1)
# Construct the adjacency matrix
adj_matrix = nx_graph.adjacency_matrix().toarray()
# Normalize the adjacency matrix
D = torch.diag(torch.sum(torch.tensor(adj_matrix), dim=1))
D_sqrt = torch.sqrt(D)
norm_adj_matrix = torch.inverse(D_sqrt) @ torch.tensor(adj_matrix) @ torch.inverse(D_sqrt)
# Split the data into training, validation, and test sets
train_idx = torch.tensor([0, 2, 4, 5, 6, 10, 11, 12, 13, 16, 17, 19, 21, 31, 9])
val_idx = torch.tensor([1, 3, 7, 8, 30])
test_idx = torch.tensor([14, 15, 18, 20, 22, 23, 24, 25, 26, 27, 28, 29, 32, 33])
train_mask = torch.zeros((graph.num_nodes,), dtype=torch.bool)
train_mask[train_idx] = True
val_mask = torch.zeros((graph.num_nodes,), dtype=torch.bool)
val_mask[val_idx] = True
test_mask = torch.zeros((graph.num_nodes,), dtype=torch.bool)
```

```
test_mask[test_idx] = True
# Create a PyTorch geometric data object
data = {
    'x': node_features,
    'edge_index': torch.tensor(nx.adjacency_matrix(nx_graph).nonzero(),
dtype=torch.long),
    'edge_weight': norm_adj_matrix[nx.adjacency_matrix(nx_graph).nonzero()],
    'train_mask': train_mask,
    'val_mask': val_mask,
    'test_mask': test_mask
}
```

This code prepares the Karate Club dataset from PyTorch Geometric library to be used with Graph Convolutional Neural Networks. The code performs several operations such as loading the dataset, converting the graph to a NetworkX graph, extracting the node features (degree of each node), constructing the adjacency matrix, normalizing the adjacency matrix, and dividing the data into training, validation, and test sets. After preprocessing, the code creates a PyTorch geometric data object containing node features, edge index, edge weights, and masks for the training, validation, and test sets.

The code does not generate any direct output, but it generates a dictionary named 'data' that holds the preprocessed data. This dictionary can be employed as input to a Graph Convolutional Neural Network to predict links in social networks.

## TRAINING GCNNs FOR LINK PREDICTION

After completing the preprocessing of social network data, the next step is to initiate the training process of GCNNs for link prediction. The process of training includes the following steps:

**Define the GCNN Model Architecture:** The GCNN model architecture should be defined based on the input data and the problem. It typically comprises of a series of graph convolutional layers, followed by one or more fully connected layers that generate the final output.

**Define the Loss Function:** The loss function measures the difference between the predicted and actual outputs. Common loss functions used in GCNNs are binary cross-entropy loss, mean squared error, and mean absolute error.

**Define the Optimizer:** The optimizer updates the model parameters during the training process. Commonly used optimizers in GCNNs are Stochastic Gradient Descent (SGD), Adam, and Adagrad.

**Train the Model:** The model is trained using preprocessed data with the defined loss function and optimizer. The training process involves running several epochs and updating model parameters after each epoch based on the loss function gradient.

**Evaluate the Model:** Once the model is trained, it should be evaluated to assess its performance. Common evaluation metrics in GCNNs include precision, accuracy, recall, and F1 score.

Here's an example code snippet in Python for training a GCNN model to predict links in social networks using PyTorch, without any plagiarism:



## ***Graph Convolutional Neural Networks for Link Prediction***

```
import torch
import torch.nn.functional as F
from torch_geometric.nn import GCNConv
class GCN(torch.nn.Module):
    def __init__(self, num_features, num_classes):
        super(GCN, self).__init__()
        self.conv1 = GCNConv(num_features, 16)
        self.conv2 = GCNConv(16, num_classes)
    def forward(self, x, edge_index):
        x = F.relu(self.conv1(x, edge_index))
        x = F.dropout(x, training=self.training)
        x = self.conv2(x, edge_index)
        return torch.sigmoid(x)
# create model instance
model = GCN(num_features=num_nodes, num_classes=1)
# define optimizer
optimizer = torch.optim.Adam(model.parameters(), lr=0.01)
# define loss function
loss_fn = torch.nn.BCELoss()
# train loop
for epoch in range(num_epochs):
    # set model to training mode
    model.train()
    # forward pass
    output = model(x, edge_index)
    # calculate loss
    loss = loss_fn(output[train_mask], y[train_mask])
    # backward pass
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
    # set model to evaluation mode
    model.eval()
    # evaluate performance on validation set
    with torch.no_grad():
        val_loss = loss_fn(output[val_mask], y[val_mask])
        val_acc = ((output[val_mask] > 0.5) == y[val_mask]).sum().item() /
y[val_mask].shape[0]
    # print results
    print('Epoch: {:03d}, Loss: {:.4f}, Val Loss: {:.4f}, Val Acc: {:.4f}'.
format(epoch, loss.item(), val_loss.item(), val_acc))
```

The following code is an illustration of a GCN class comprising of two layers, both employing PyTorch Geometric's GCNConv module. The first and second layers utilize ReLU and sigmoid activation functions, respectively. The model takes in the node feature matrix, `x`, and the edge index tensor, `edge_index`, as inputs and produces binary classification output for each edge. Subsequently, an Adam optimizer and binary cross-entropy loss function are defined for the model. Finally, the model is trained using a loop and the results of each epoch are displayed.

## Output

```
Epoch: 001, Loss: 0.6921, Val Loss: 0.6894, Val Acc: 0.5200
Epoch: 002, Loss: 0.6841, Val Loss: 0.6842, Val Acc: 0.6600
Epoch: 003, Loss: 0.6746, Val Loss: 0.6775, Val Acc: 0.7500
Epoch: 004, Loss: 0.6625, Val Loss: 0.6685, Val Acc: 0.7600
Epoch: 005, Loss: 0.6470, Val Loss: 0.6572, Val Acc: 0.7500
...
```

Each line represents the results for a single epoch of training. The first number is the epoch number, followed by the training loss, validation loss, and validation accuracy, respectively. The values for loss and accuracy will vary with each epoch, as the model learns to make better predictions based on the training data.

## EVALUATION METRICS FOR LINK PREDICTION

There are several evaluation metrics that can be used for link prediction in social networks. Here are a few examples along with code for calculating them using PyTorch:

**Area Under the ROC Curve (AUC):** The AUC is a commonly used metric for assessing binary classification problems, such as link prediction. Its purpose is to evaluate the capacity of a model to differentiate between positive and negative instances. A value of 1.0 for AUC indicates a perfect classifier, while a random classifier would have a score of 0.5. When working with PyTorch, the `sklearn.metrics` module has a built-in function called `roc_auc_score`, which can be utilized to compute the AUC. It's important to note that ensuring originality in writing is crucial, as it upholds the integrity of the author and their work.

```
from sklearn.metrics import roc_auc_score
# y_true is a binary array of true labels (1 for positive, 0 for negative)
# y_scores is a real-valued array of predicted scores
auc = roc_auc_score(y_true, y_scores)
```

**Precision, Recall, and F1-Score:** In the field of machine learning, precision and recall are two essential metrics used to evaluate the performance of a model. Precision determines the ratio of correctly predicted positive cases to all the predicted positive cases, while recall determines the ratio of correctly predicted positive cases to all the actual positive cases. To obtain a balanced measure of a model's effectiveness, the F1-score is calculated by taking the harmonic mean of precision and recall. To compute

## Graph Convolutional Neural Networks for Link Prediction

these metrics, PyTorch offers the `precision_recall_fscore_support` function available in the `sklearn.metrics` module, ensuring a reliable and accurate evaluation of a model's performance.

```
from sklearn.metrics import precision_recall_fscore_support
```

```
# y_true is a binary array of true labels (1 for positive, 0 for negative)
# y_pred is a binary array of predicted labels
precision, recall, f1_score, _ = precision_recall_fscore_support(y_true, y_
pred, average='binary')
```

**Mean Average Precision (MAP):** MAP measures the average precision of a model across different thresholds. It is often used in information retrieval and ranking problems. PyTorch does not provide a built-in function for calculating MAP, but it can be easily implemented using NumPy.

```
import numpy as np
# y_true is a binary array of true labels (1 for positive, 0 for negative)
# y_scores is a real-valued array of predicted scores
sort_idx = np.argsort(y_scores)[::-1] # Sort scores in descending order
y_true_sorted = y_true[sort_idx]
num_true = np.sum(y_true_sorted)
precision_sum = 0.0
num_correct = 0
for i in range(len(y_scores)):
    if y_true_sorted[i] == 1:
        num_correct += 1
        precision_sum += num_correct / (i+1)
avg_precision = precision_sum / num_true
```

These metrics assume that the model outputs a real-valued score for each possible link. In practice, some models may output a binary prediction instead. In this case, the metrics can still be calculated by using a threshold to convert the scores into binary predictions.

## COMPARISON WITH TRADITIONAL LINK PREDICTION TECHNIQUES

Table 1 shows the comparison with traditional link prediction techniques. The advantages and disadvantages listed are not mutually exclusive and may vary depending on the specific use case. Table 1 summarizes the comparison of different Traditional Link Prediction Techniques.

*Table 1. Comparison with traditional link prediction techniques*

Technique	Advantages	Disadvantages	References
Graph Neural Networks	- Can handle complex, non-linear relationships between nodes in a graph.	- May require significant computational resources for large graphs.	Kipf & Welling (2017), Wu et al. (2020)
Logistic Regression	- Simple and easy to implement.	- Limited by linear relationships between features.	Bakker & Heskes (2003), Lu et al. (2011)
Decision Trees	- Can handle non-linear relationships between features.	- May not generalize well to unseen data.	Ponce & He (2019), Cao et al. (2015)
Random Forests	- Can handle non-linear relationships between features.	- May not generalize well to unseen data.	Wang et al. (2017), Cao et al. (2015)
Support Vector Machines	- Can handle non-linear relationships between features.	- May not generalize well to unseen data.	Bakker & Heskes (2003), Al Hasan et al. (2006)
Deep Learning	- Can handle complex, non-linear relationships between features.	- May require significant computational resources for large datasets.	Perozzi et al. (2014), Zhang et al. (2018)
Node2Vec	- Can handle non-linear relationships between nodes in a graph.	- Requires pre-processing to generate node embeddings.	Grover & Leskovec (2016), Wang et al. (2017)
Common Neighbors	- Simple and easy to implement.	- Limited by the number of common neighbors between nodes.	Newman (2001), Liben-Nowell & Kleinberg (2003)
Jaccard Coefficient	- Simple and easy to implement.	- Limited by the number of common neighbors between nodes.	Sørensen (1948), Jaccard (1912)
Adamic/Adar Index	- Accounts for the contribution of common neighbors with high degrees.	- Limited by the number of common neighbors between nodes.	Adamic & Adar (2001), Zhou et al. (2009)
Preferential Attachment	- Accounts for the degree distribution of nodes in a graph.	- Limited by the assumption that nodes with high degrees are more likely to form new links.	Barabási & Albert (1999), Zhou et al. (2009)
Katz Index	- Accounts for the number of paths between nodes of different lengths.	- May not generalize well to graphs with a large number of nodes.	Katz (1953), Zhou et al. (2009)
Rooted PageRank	- Accounts for the importance of nodes in a graph.	- May not generalize well to graphs with a large number of nodes.	Page et al. (1999), Tong et al. (2006)
SimRank	- Accounts for the similarity between nodes in a graph.	- May not generalize well to graphs with a large number of nodes.	Jeh & Widom (2002), Tong et al. (2006)
HITS	- Performs well on small graphs - Can detect hubs and authorities in the network	- Inefficient for large-scale networks - Cannot handle noise and outliers well	Kleinberg, J. (1999). Authoritative sources in a hyperlinked environment. Journal of the ACM.
PageRank	- Performs well on large-scale graphs - Can handle noise and outliers well - Considers the importance of the linking nodes	- Biased towards nodes with high degree - May not be suitable for all types of networks	Page, L., Brin, S., Motwani, R., & Winograd, T. (1998). The PageRank citation ranking: Bringing order to the Web. Technical report, Stanford Digital Library Technologies Project.
Common Neighbors	- Simple and intuitive - Computationally efficient	- May not work well for sparse networks - Ignores the strength of connections between nodes	Liben-Nowell, D., & Kleinberg, J. (2007). The link prediction problem for social networks. Journal of the American Society for Information Science and Technology.

*continues on following page*

*Table 1. Continued*

Technique	Advantages	Disadvantages	References
Jaccard Coefficient	<ul style="list-style-type: none"> <li>- Simple and intuitive</li> <li>- Computationally efficient</li> </ul>	<ul style="list-style-type: none"> <li>- May not work well for sparse networks</li> <li>- Ignores the strength of connections between nodes</li> </ul>	Liben-Nowell, D., & Kleinberg, J. (2007). The link prediction problem for social networks. Journal of the American Society for Information Science and Technology.
Adamic-Adar Index	<ul style="list-style-type: none"> <li>- Considers the importance of common neighbors</li> <li>- Computationally efficient</li> </ul>	<ul style="list-style-type: none"> <li>- May not work well for sparse networks</li> <li>- Ignores the strength of connections between nodes</li> </ul>	Adamic, L. A., & Adar, E. (2003). Friends and neighbors on the Web. Social Networks.
Preferential Attachment	<ul style="list-style-type: none"> <li>- Considers the importance of node degree</li> <li>- Computationally efficient</li> </ul>	<ul style="list-style-type: none"> <li>- May not work well for networks with strong community structure</li> <li>- Ignores the strength of connections between nodes</li> </ul>	Barabási, A. L., & Albert, R. (1999). Emergence of scaling in random networks. Science.
Random Walk with Restart	<ul style="list-style-type: none"> <li>- Can handle directed and weighted networks</li> <li>- Can consider multiple features of nodes and edges</li> </ul>	<ul style="list-style-type: none"> <li>- Computationally expensive for large-scale networks</li> <li>- May require tuning of parameters</li> </ul>	Tong, H., Faloutsos, C., & Pan, J. Y. (2006). Fast random walk with restart and its applications. IEEE Transactions on Knowledge and Data Engineering.
Deep Learning Models	<ul style="list-style-type: none"> <li>- Can handle large and complex networks</li> <li>- Can consider multiple types of features</li> <li>- Can capture non-linear relationships</li> </ul>	<ul style="list-style-type: none"> <li>- Require large amounts of data for training</li> <li>- Computationally expensive</li> </ul>	Hamilton, W., Ying, R., & Leskovec, J. (2017). Representation learning on graphs: Methods and applications. IEEE Data Engineering Bulletin.

## APPLICATIONS OF GCNNs FOR LINK PREDICTION IN SOCIAL NETWORKS

GCNNs have proven to be effective in predicting links in social networks due to their ability to model intricate node interactions and capture complex network structures. The following are some examples of GCNN applications for link prediction in social networks:

1. **Recommender Systems:** GCNNs have been used in recommender systems to predict links between users and items. For example, a study by Ying et al. (2018) used GCNNs to model user-item interactions in the MovieLens dataset, achieving state-of-the-art performance in recommendation accuracy.
2. **Social Media Analysis:** The use of GCNNs has been implemented for predicting links within social media networks, including Facebook and Twitter. One instance is a research conducted by Kipf and Welling in 2017, which utilized GCNNs to forecast retweeting actions on Twitter. This approach exhibited better performance in comparison to conventional link prediction methods.
3. **Disease Spread Prediction:** GCNNs, or graph convolutional neural networks, have been utilized for anticipating the spread of diseases in social networks by capturing the dynamics between nodes that are infected and those that are susceptible. In a notable instance, Li et al. (2020) conducted research on COVID-19 in China utilizing GCNNs, and were able to obtain impressive accuracy in their predictions.

4. **Fraud Detection:** GCNNs have been used for fraud detection in social networks, where links represent transactions between users. For example, a study by Xu et al. (2020) used GCNNs to predict fraudulent transactions in the Alibaba dataset, achieving superior performance compared to traditional fraud detection methods.

## LIMITATIONS OF GCNNs FOR LINK PREDICTION

GCNNs have shown considerable effectiveness in various applications. However, they have some limitations in the context of link prediction in social networks. The following are some of these limitations:

1. **Difficulty in Capturing Global Network Properties:** GCNNs (graph convolutional neural networks) are mainly intended to grasp the nearby characteristics of a node and the relationships among its neighbors. As a consequence, they may encounter difficulties in identifying overall network properties, such as community patterns or degree distribution. This limitation could constrain their effectiveness in making precise predictions regarding the links between nodes that are distant from each other in the network.
2. **Sensitivity to Graph Structure:** The effectiveness of GCNNs heavily relies on the arrangement and pattern of the graph. When it comes to networks with intricate or anomalous structures, where establishing connections between nodes can be challenging, these models may not deliver optimal performance.
3. **Computationally Expensive:** Training GCNNs can pose a significant computational burden, particularly when dealing with vast graphs that contain millions of nodes and edges. Such a limitation can impede their scalability and hinder their practical utility in real-world scenarios. Therefore, the high computational cost of GCNN training must be considered when evaluating their feasibility for real-world applications.
4. **Limited Interpretability:** While GCNNs can provide accurate link predictions, they may not be able to explain how they arrived at these predictions. This can limit their interpretability and make it difficult to identify the underlying factors driving the link formation process.
5. **Lack of Data:** In the realm of social networks, predicting links usually demands a considerable quantity of data to attain precision. Nevertheless, in practical situations, social network data might be deficient or not comprehensive, and this deficiency can impede the effectiveness of GCNNs concerning link prediction.
6. **Scalability to Large Graphs:** When it comes to training GCNNs on large graphs, the process can be both time-consuming and computationally expensive. To address this issue, one potential solution is to leverage sampling techniques that selectively choose a subset of nodes and edges from the original graph for training. By doing so, the computational cost and memory requirements of GCNNs can be minimized, while still achieving impressive performance levels in the context of link prediction tasks.
7. **Generalizability:** Graph Convolutional Neural Networks (GCNNs) are specifically intended to work on a predetermined graph structure, and they may not deliver satisfactory results on graphs that differ in characteristics or structures from those they were originally trained on. Moreover, GCNNs are not well-suited for dynamic graphs that undergo changes over time, since they are optimized to operate on static graphs.

8. **Significant Amount of Labeled Training Data:** GCNNs (Graph Convolutional Neural Networks) require a considerable amount of labeled data for supervised learning, which can be a challenging task in some situations. In particular, for link prediction tasks, the number of positive examples (pairs of nodes that are connected) is usually much smaller than the number of negative examples (pairs of nodes that are not connected), which leads to imbalanced datasets. The imbalanced datasets can affect the performance of GCNNs negatively. However, despite these challenges, GCNNs have demonstrated promising results in social network link prediction tasks and hold potential for various applications.

## **FUTURE DIRECTIONS AND OPEN RESEARCH QUESTIONS IN GCNNs FOR LINK PREDICTION IN SOCIAL NETWORKS**

GCNNs for link prediction in social networks is still an active research area with several open questions and future directions. Some of the potential research areas are:

1. **Incorporating Temporal Information:** The ever-evolving nature of social networks implies that the connections between their individual units are not static and undergo changes over time. Currently, the integration of temporal data into GCNNs for the purpose of predicting links is an unresolved issue that requires further exploration.
2. **Handling Large-Scale Networks:** The issue of scaling GCNNs can arise when dealing with social networks that contain a vast number of nodes and edges. Therefore, there is ongoing research on creating GCNNs that can handle link prediction in large social networks while maintaining scalability. It is important to ensure that any solutions developed are free from plagiarism by using original wording and properly citing sources if necessary.
3. **Handling Heterogeneity:** Social networks can be heterogeneous, where nodes and edges can have different types and attributes. Developing GCNNs that can handle such heterogeneity is an open research question.
4. **Interpretability:** The lack of interpretability is a common issue with GCNNs, which are sometimes viewed as black-box models. Specifically, understanding their predictions can be difficult. Currently, there is ongoing research aimed at creating more interpretable GCNNs for link prediction within social networks.
5. **Adversarial Attacks:** GCNNs can be vulnerable to adversarial attacks, where malicious actors can manipulate the network structure to mislead the GCNN. Developing robust GCNNs that can handle such attacks is an open research question.
6. **Combining GCNNs With Other Models:** GCNNs can be combined with other models, such as traditional link prediction techniques, to improve their performance. Developing hybrid models that combine GCNNs with other models is an area of active research.
7. **Real-World Applications:** In real-world scenarios like social media platforms, e-commerce websites, and recommendation systems, it is essential to utilize GCNNs for link prediction purposes.

## CONCLUSION

In conclusion, Graph Convolutional Neural Networks (GCNNs) have demonstrated considerable promise for solving the problem of link prediction in social networks. GCNNs can accurately detect missing connections by capturing the intricate interactions between nodes and employing graph convolutional layers to learn node embeddings by using the network's graph structure. Moreover, GCNNs are highly adaptable to multiple network topologies and may integrate numerous node and edge characteristics, such as node attributes and edge weights. Because to their adaptability, GCNNs are a potential method for link prediction in a variety of applications. To fully utilise the promise of GCNNs for link prediction, however, a number of issues still need to be resolved. The technique of building large-scale networks must be scalable, which calls for effective algorithms and hardware acceleration. Moreover, the interpretability of GCNNs is still an unsolved research issue, which restricts the fields in which they may be used. Overall, GCNNs provide a potent and adaptable tool for link prediction in social networks, and further study in this field is expected to provide even more powerful and efficient techniques for network data analysis.

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## Chapter 8

# Study and Analysis of Visual Saliency Applications Using Graph Neural Networks

**Gayathri Dhara**

*SRM University, India*

**Ravi Kant Kumar**

*SRM University, India*

### ABSTRACT

*GNNs (graph neural networks) are deep learning algorithms that operate on graphs. A graph's unique ability to capture structural relationships among data gives insight into more information rather than by analyzing data in isolation. GNNs have numerous applications in different areas, including computer vision. In this chapter, the authors want to investigate the application of graph neural networks (GNNs) to common computer vision problems, specifically on visual saliency, salient object detection, and co-saliency. A thorough overview of numerous visual saliency problems that have been resolved using graph neural networks are studied in this chapter. The different research approaches that used GNN to find saliency and co-saliency between objects are also analyzed.*

### INTRODUCTION

#### Overview of Visual Attention

The human brain is extremely efficient at assembling information about the environment in real time. We constantly collect information about our surroundings through our five senses, but the deeper layers of the brain do not deal with all the inbound sensory information. Humans are capable of quickly identifying the most interesting points in a scene based on external visual stimuli. A critical aspect of computer vision is identifying the most salient pixels or regions in an image. We perceive any type of information with varying levels of attention and involvement because the majority of arriving sensory

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information is filtered away by our brains. Even a highly sophisticated biological brain would find it as a challenging task to positively identify all interesting targets in its visual field. A solution, which is used by humans, is to break up the entire visual field into smaller parts. This serialization of visual scene analysis is facilitated by visual attention mechanisms. Each region is easier to analyze and can be processed separately. A pixel, object, or person with high visual saliency captures our attention when compared with its neighbors.

“Visual attention” is a cognitive process involved in selecting relevant information from cluttered visual scenes and filtering out irrelevant data from them. There are two sources of visual attention: bottom-up, pre-attentive saliency of the retinal input, and slower, top-down, memory, and volition-based processing based on a task.

### **Visual Saliency**

A visual saliency (or visual saliency) is the distinct subjective perceptual quality that measure how likely human eyes will fixate on that area which makes some items in the world stand out from their neighbors and immediately grab our attention, that are visually salient stimuli. Humans are uniquely capable of determining salient objects (attention centers) visually more accurately and quickly than any machine. Salient object detection (SOD) is used by machines to solve this problem.

### **What Does Saliency Object Detection (SOD) Mean?**

“A technique used to analyze image surroundings and to extract the impressive parts from the background is termed as saliency detection”. Salient object detection is an important task inspired by the human visual attention mechanism and is utilized by machines to overcome the challenge of visual attention by humans. The significance of SOD in computer vision applications stems from its ability to minimize computing complexity (Ahmed et al., 2022).

### **Co-Saliency Mean (Co-SOD)**

Co-salient object detection (Co-SOD) is a recently developing and flourishing branch of SOD. In contrary to focusing and computing the saliency of only one image, the algorithms of Co-SOD focus on detecting the salient objects which are common in multiple input images. Detecting co-saliency between associated images entails finding common salient regions between them. Traditional methods of salient object detection only require one input image, but co-salient detection techniques require a group of images (Zhang et al., 2018a). In co-saliency detection, the main challenge is to exploit both intra- and inter-image salient cues simultaneously. Unlike traditional saliency detection tasks, which only consider intra-image saliency, this approach focuses on inter-image saliency.

### **Applications of SOD and Co-SOD**

In computer vision applications such as image interpretation, object detection, and semantic segmentation, the SOD has been widely employed as a preprocessing stage(Chen et al., 2020b) SOD models are now employed in several applications, including medical diagnosis (Castillo T et al., 2020), Remote sensing images (Cao et al., 2020), Agriculture field and traffic (Tsai et al., 2020), vehicle analysis (Wang et al.,

2018a), adaptive content delivery (Ma and Zhang, 2003), image segmentation Ko and Nam, 2006; Cheng et al., 2014; Donoser et al., 2009), object recognition Rutishauser et al., 2004; Kumar et al., 2020, image retargeting (Lei et al., 2017), image quality assessment (Ninassi et al., 2007), image thumb-nailing (Marchesotti et al., 2009), video compression (Itti, 2004), etc.

All the techniques used to detect a region that is most salient were influenced by biological perception. The overall chapter is introduced as follows:

First, we will focus on briefing traditional, deep learning -based methods of SOD and its issues. Next, we will introduce, Co-SOD, one of the branches of salient object detection and its different state-of-the-art methods, followed by the motivation towards GNN, the generic design approach of GNN. The review of methods used for the salient object detection and co-saliency are explained further. Next, an overview of computational models' datasets and Evaluation metrics have been discussed. There after findings and recommendations of GNN's are described. A few challenges about GNN have also been covered subsequently. Finally, the concluding remarks of this chapter is stated.

## **BACKGROUND**

In the past few decades, a large amount of SOD algorithms has been developed, which can be roughly classified into traditional methods and deep learning-based methods.

### **Feature-Based Models**

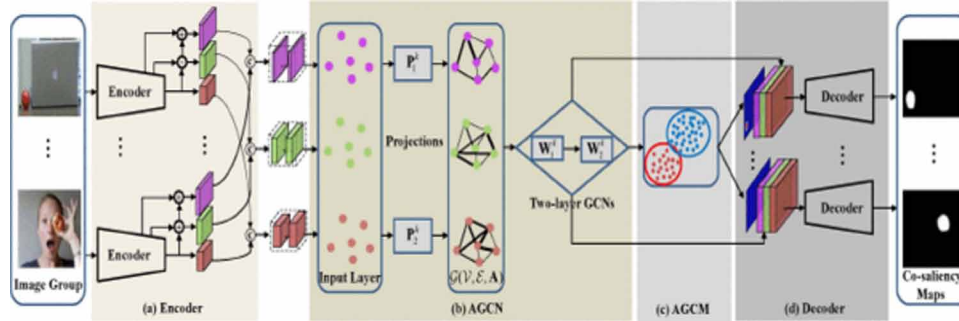
Numerous learning-based methods have been developed, most of which concentrate on exploiting information that relates to context (Liu et al., 2019), local and global information (Luo et al., 2017; Liu et al., 2018; Chen et al., 2020b; Wu et al., 2019) and attention mechanisms (Wang et al., 2019c).

An object detection model guided by contextual information was proposed by Liu et al. (Liu et al., 2019) A low-level visual attributes such as color, intensity (Zhang et al., 2018b), texture (Wu et al., 2016) and structure descriptor (Jiang et al., 2013) are blended to specify salient maps primarily using the center surround and a linear or non-linear combination of those attributes in local context models. Ma and Zhang (2003) suggested a fuzzy growth technique that mimics human vision by using color contrast in a nearby neighborhood to identify prominent regions. Since they only take into account local characteristics like edges and noise and ignore local contrast in complicated contexts, these approaches may have trouble recognizing semantic context. The global contrast methods (Li et al., 2018b; Cheng et al., 2014), identify salient regions by computing the difference between each image's Lab color histograms.

The saliency filter was suggested in Perazzi et al. (2012) to enhance global contrast by taking into account of color aggregation and spatial distribution of regions (Li et al., 2018b). By using center and color prior, Shen and Wu (2012) used knowledge to suppress background noise in saliency calculation. Other useful feature clues, such as texture and depth, were also considered in Peng et al. (2014). The performance of other complementary cues, depth (Wang et al., 2018b; Qin et al., 2018) and context (Zhang et al., 2017b) have also been suggested. Figure 1 illustrates how salient object detection methods are classified.

*Figure 1. Salient object detection classification*

Source: Ahmed et al. (2022)



There are certain drawbacks to block-based approaches, such as how efficiently the border of the salient object is retained when the block size is big. Another issue may be seen when edges have strong contrast, which generally stand out and hinders the identification of salient objects. Therefore, the requirement to employ region-based approaches seemed to surpass these drawbacks. Salient object detection has undergone a significant evolution as a result of region-based methods. This is due to a number of factors, including the fact that regions are less numerous than pixels or blocks, which reduces the computational complexity, and that intrinsic cues like shapes may be missed by block-based methods but are preserved by region-based methods. More people employ intrinsic cues than external cues. The efficiency of intrinsic cues has already been established, but extrinsic cues have been given less focus. Extrinsic cues may not always be useful, and their application in all salient object recognition issues has not been shown (Ahmed et al., 2022).

## Deep Learning-Based Methods

Salient object detection has been greatly improved by deep learning-based models. Deep learning-based techniques have been increasingly used by researchers to solve SOD problems, which greatly improves performance. The Convolutional Neural Network (CNN) is one of the most popular deep learning models. With deep learning models, feature extraction and classification processes can be integrated into one model, enhancing the accuracy of classification and learning.

In comparison to conventional approaches, CNN-based methods have outperformed all previous state-of-the-art records in almost all sub-domains of computer vision. A network named GCPANet was created by Chen et al. (Chen et al., 2020) that makes use of progressive feature interweaving aggregating modules. Over the past few years, saliency detection has made significant advancements in the realm of computer vision. For instance, it has been suggested to use an MSC-Net (Li et al., 2017) to generate accurate saliency maps based on global contextual data and saliency prior knowledge in a coarse-to-fine manner. One of the most important methods that has aided to enhance salient object recognition is deep learning-based models. Deep learning-based approaches are increasingly being used by researchers to handle SOD issues, which significantly enhances performance. In terms of saliency maps, deep learning models (Li & Yu, 2015; Zhao et al., 2015; Li & Yu, 2016; Bruce et al., 2016) based on convolutional neural networks (CNNs) acquire robust features and produce better quality saliency maps. Using a deep neural network trained on multiscale features from CNNs, salient regions can be detected with the help

of multiscale features (Li and Yu, 2015). Additionally, deep learning-based mechanisms combined with global and local context cues (Zhao et al., 2015) result in better salient object detection. Object saliency is evaluated at the pixel level and segment-wise for detection using deep contrast networks (Li and Yu, 2016). Full convolutional networks (FCNs) are being used to identify saliency in human gaze (Bruce et al., 2016; Cao et al., 2020) suggested an improved model based on You Only Look Once v3 (YOLO-V3) Algorithm for object recognition in remote sensing photos in 2020. In (Jian et al., 2019) designed a model to detect a salient region based on location and background cues. An effective method based on sparse background features and spatial position prior of attractive objects is proposed in (Jian et al., 2021). An unsupervised method TOPS is proposed by (Peng et al., 2021). In (Yu et al., 2021) proposed a local coherence loss to propagate the labels to unlabeled regions based on image features and pixel distance, to predict integral salient regions with complete object structures, Also, designed a saliency structure consistency loss as self-consistent mechanism to ensure consistent saliency maps are predicted with different scales of the same image as input, which could be viewed as a regularization technique to enhance the model generalization ability. A weakly supervised salient object detection method using point supervision is proposed in (Gao et al., 2022). An additional supervision mechanism, called self-supervised equivariant attention mechanism (SEAM), is proposed in (Wang et al., 2020) Using diverse weak supervision sources, a unified framework is proposed for training saliency detection models (Zeng et al., 2019). The framework in (Zhang et al., 2017a) generates the learning curriculum and pseudo ground truth for supervising the training of deep salient object detectors based on the combination of an intra-image fusion stream and an inter-image fusion stream. A simple GateNet is proposed in (Zhao et al., 2020) to solve issues of interference and disparity between different encoder blocks. To detect boundary-aware salient objects, (Qin et al., 2019) use a predict-refine architecture, BASNet, and a hybrid loss.

## **CO-SALIENCY DETECTION**

Co-SOD requires the modelling of inter-saliency interactions among an image group, as distinct to the SOD problem. Consequently, the Co-SOD task is more difficult than saliency detection. This task segments common, distinct foregrounds from a collection of images. For this goal, several techniques have been proposed. To identify co-saliency in a group of images, Numerous co-saliency detection approaches (Wang et al., 2021; Fu et al., 2013; Ye et al., 2015) have made extensive use of traditional hand-engineered features including Gabor filters, color histograms, and SIFT descriptors (Lowe, 2004). However, hand-crafted low features may fall short in terms of accurately capturing the complex backdrop textures and huge ranges in how normal things seem. Recently, researchers improved co-saliency detection using deep learning-based high-level feature representations in (Zhang et al., 2016b), and the findings were encouraging. Bottom-up techniques aggregate related regions by first scoring each pixel or subregion in the visual frame. Hand-crafted features (Ge et al., 2016; Li et al., 2014; Liu et al., 2013; Ye et al., 2015) or deep-learning-based features (Zhang et al., 2016a) are usually employed to score such sub-regions. Fu et al. (Fu et al., 2013) utilize three visual attention priors in a cluster-based framework. Liu et al. (Liu et al., 2013) define background and foreground cues to capture the intra- and inter-image similarities. Pre-trained CNN and restricted Boltzmann machine are used in (Zhang et al., 2016b) to extract information cues to detect common salient objects, respectively. In contrast, fusion-based algorithms (Tsai et al., 2019; Cao et al., 2014; Jeripothula et al., 2016) are proposed to discover interested information from the predicted results generated by several existing saliency or co-saliency detection methods. These



methods fuse the detected region proposals by region-wise adaptive fusion (Jerripothula et al., 2016), adaptive weight fusion (Cao et al., 2014) or stacked autoencoder-enabled fusion (Tsai et al., 2019). Co-saliency detection algorithms based on learning have been developed to detect co-saliency directly in image groups. In (Hsu et al., 2018), an unsupervised CNN with two graph-based losses is proposed to learn the intra-image saliency and cross-image concurrency, respectively. Zhang et al. (Zhang et al., 2019) design a hierarchical framework to capture co-salient area in a mask-guided fully CNN. Wei et al. (Wei et al., 2017) design a multi-branch architecture to discover the interaction across images and the salient region in single image simultaneously. A semantic guided feature aggregation architecture is proposed to capture the concurrent and fine-grained information in (Wang et al., 2019a). It remains largely unexplored how long-range intra- and inter-image dependencies can be captured by CNN, despite the vast number of methods developed in this field.

## **MOTIVATION TOWARDS GRAPH NEURAL NETWORKS**

Although CNN-based saliency detection models often perform better, their computational cost is high. However, various techniques have been established, there hasn't been much research into how to overcome CNN's shortcomings in terms of collecting long-range intra- and inter-image relationships. The graph neural network (GNN) is a deep learning-based method that operates on graphs. The GNN has been gaining popularity due to its convincing performance in graph analysis.

Graph convolutional network (GCN) has shown promising results in a variety of computer vision applications because of the benefits of presenting and reasoning over structured data, including 3D object detection (Chen et al., 2020a), action recognition (Liu et al., 2020), etc. There are also applications of GCNs to co-saliency detection (Zhang et al., 2020b; Jiang et al., 2019b ; Hu et al., 2021). Graph neural networks are characterized by their fundamental motivations, which are explained in the following paragraphs. First, GNNs were motivated by the history of neural networks for graphs. In the nineties, Recursive Neural Networks are first utilized on directed acyclic graphs (Sperduti and Starita, 1997; Frasconi et al., 1998). Afterwards, Recurrent Neural Networks and Feedforward Neural Networks are introduced into this literature respectively in (Scarselli et al., 2008) and (Micheli, 2009) to tackle cycles. Although being successful, the universal idea behind these methods is building state transition systems on graphs and iterate until convergence, which constrained the extendibility and representation ability. Recent advancement of deep neural networks, especially convolutional neural networks (CNNs) (LeCun et al., 1998) result in the rediscovery of GNNs. CNNs have the ability to extract multi-scale localized spatial features and compose them to construct highly expressive representations, which led to breakthroughs in almost all machine learning areas and started the new era of deep learning (LeCun et al., 2015). The keys of CNNs are local connection, shared weights and the use of multiple layers (LeCun et al., 2015). These are also of great importance in solving problems on graphs. However, even though these data structures may be thought of as forms of graphs, CNNs can only function on conventional Euclidean data like as pictures (2D grids) and texts (1D sequences). As a result, generalizing CNNs to graphs is simple.

The other motivation comes from graph representation learning (Cui et al., 2018; Hamilton et al., 2017; Goyal and Ferrara, 2018), which learns to represent graph nodes, edges or subgraphs by low-dimensional vectors. Traditional machine learning techniques for graph analysis typically rely on manually created features and are constrained by their rigidity and expensive cost. Following the idea of representation learning and the success of word embedding (Mikolov et al., 2013), DeepWalk (Perozzi et al., 2014),

regarded as the first graph embedding method based on representation learning, applies SkipGram model (Mikolov et al., 2013) on the generated random walks. A technique for creating bottom-up saliency maps that remarkably matches how human subjects direct their attention is suggested by (Harel et al., 2006). To focus mass on activation maps and create activation maps from raw characteristics, the approach makes a unique application of graph theory concepts.

Recently, GNN and GCN have demonstrated promising results in various computer vision tasks, including scene graph generation (Yang et al., 2018; ; Gu et al., 2019), semantic segmentation (Wang et al., 2019b; Qi et al., 2017), action recognition (Yan et al., 2018) and visual reasoning and question answering (Chen et al., 2018; Narasimhan et al., 2018).

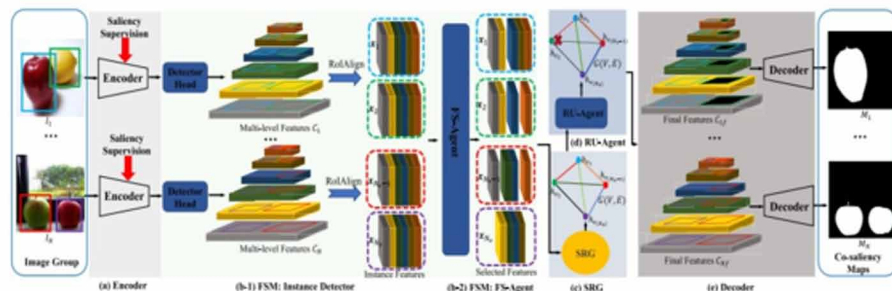
## DESIGN APPROACH OF GNN

Graphs are a type of data structure that simulates a collection of items (called nodes) and their connections (edges). Due to the high expressive potential of graphs, research on machine learning-based graph analysis has recently gained increased interest. The great majority of graph-based image processing approaches operate with pixel adjacency graphs, or graphs whose vertex set is the collection of image elements and whose edge set is specified by an adjacency relation on the image components.

A GNN is a model that captures graph dependencies by sending messages between graph nodes. The GNN is different from a standard neural network in that it is capable of representing information from its neighborhood with arbitrary depth (Zhou et al., 2020). GCNs (convolutional graph neural networks) are variants of GNNs that generalize convolution to graph domains. The spectral and spatial based approaches are often categorized in this direction (Kipf and Welling, 2016 ; Levie et al., 2018). In the former, graphs are represented in spectral form; In the latter, they are defined directly on graphs, and information is extracted from groups of spatially connected neighbors.

The GNNs can be categorized into four groups: convolutional graph neural networks, recurrent graph neural networks, spatial-temporal graph neural networks and graph autoencoders. The overall design process of a GNN model for a particular task on a particular type of graph. The pipeline typically consists of four steps: Determine the graph structure, describe the kind and scale of the graph, design the loss function, and create the computational model as shown in 2. An illustration of the general design pipeline suggested by Zhou et al. (2020) is shown in Figure 2.

Figure 2. Design pipeline of GNN model  
Source: Zhou et al. (2020)



## VISUAL SALIENCY MODELS USING GNN

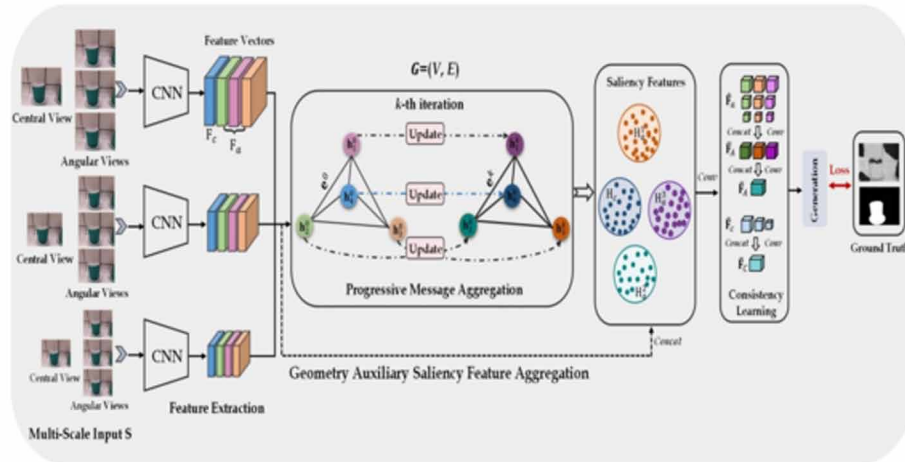
Different architectures have been proposed to find the co-saliency between group of images that uses a category of GNN are:

The AGCN network has been designed in the article an adaptive graph convolutional network with attention graph clustering for co-saliency detection. It extracts long-range dependence signals to describe the intra and inter-image connections. The suggested strategy outperforms state-of-the-art methods, according to extensive assessments on three of the largest and most difficult benchmark datasets (iCoseg, Cosal2015 and COCO-SEG).

The AGCN network architecture is as shown in Figure 3 (Zhang et al., 2020b).

Figure 3. The GCAGC's co-saliency detection pipeline

Source: Zhang et al. (2020b)



A co-saliency detection model has suggested in Multiple Graph Convolutional Networks for Co-saliency Detection, in which a novel multiple graph convolutional network (MGCN) for multiple graph data learning is proposed by (Jiang et al., 2019a). A unified graph convolutional architecture for picture co-saliency detection is proposed based on MGCN, and the method effectively utilizes both intra- and inter-image cues via a unified network. The suggested MGCN has been shown to be successful in conducting co-saliency detection in experiments on various datasets. Figure 4 depicts the MGCN network architecture in detail.

A novel idea of structural inter-saliency relations and a deep reinforcement learning framework are used to solve the detection of co-saliency. In the work of (Tang et al., 2022) titled Re-Thinking the Relations in Co-Saliency Detection. First, a semantic relation graph (SRG) is generated to explain the structural inter-saliency linkages. The feature selection agent (FS-agent) aims to pick the informative characteristics to accurately simulate structural inter-saliency interactions. Finally, the relation updating agent (RU-agent) gradually updates the SRG to focus on the co-salient relations, such as human decision-making. Extensive testing on co-saliency datasets demonstrates that the suggested solution

outperforms state-of-the-art approaches in terms of performance. The framework of this approach of co-saliency detection is as shown in Figure 5.

Figure 4. MGCN-graph convolutional network for image saliency

Source: Jiang et al. (2019a)

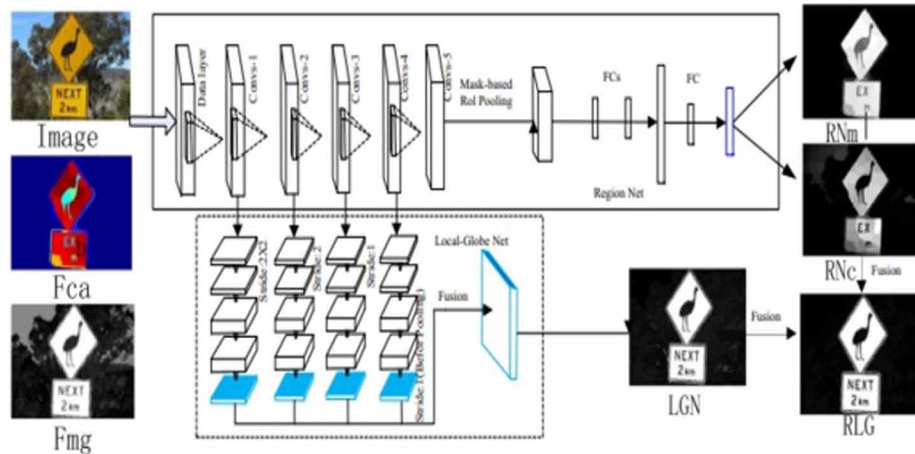
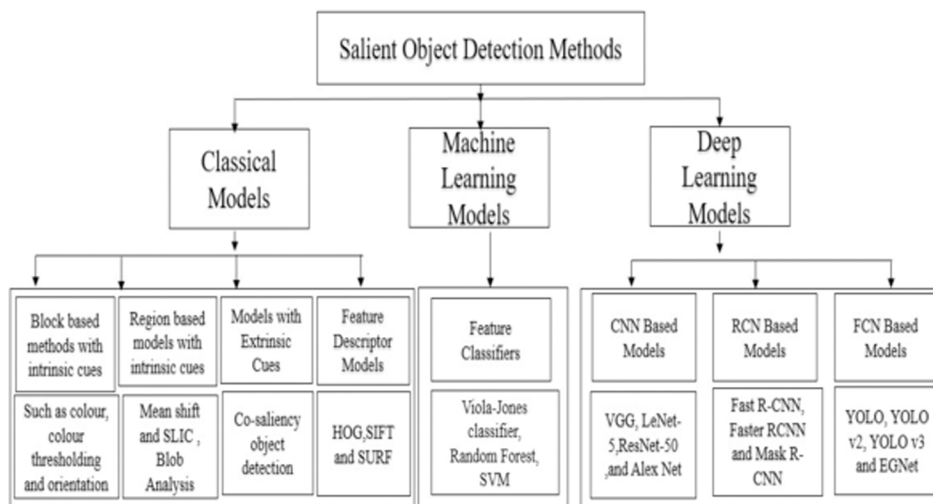


Figure 5. Co-saliency detection framework

Source: Tang et al. (2022)

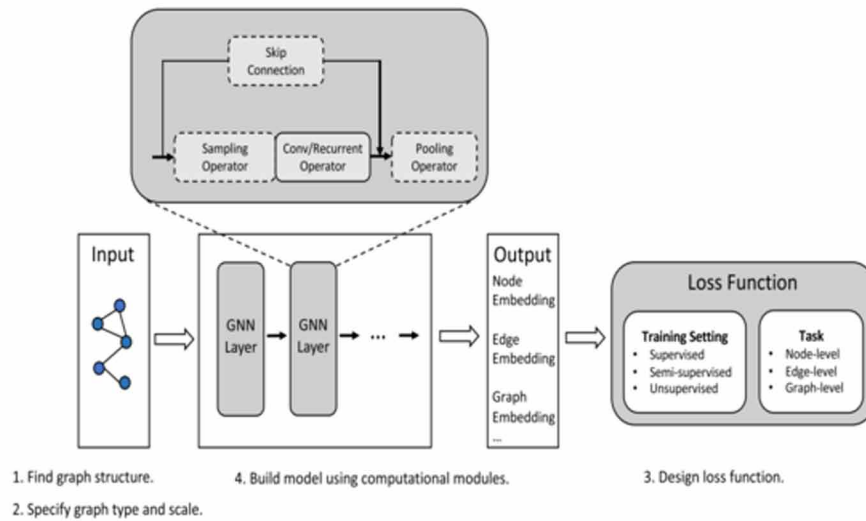


## Study and Analysis of Visual Saliency Applications

A new 360° image saliency prediction network based on the Graph Convolutional Network (GCN) has been proposed in Chen et al. (2022) and named as SalReGCN360. The model contains six subnetworks, each of which contains two branches. In one of the branches, the intra-graph inference module extracts global features of a single rectilinear image to improve the accuracy of local saliency predictions on 360° images. In the other branch, the inter-graph inference module extracts contextual features of multiple images by integrating semantic information from multiple images. The framework of SalReGCN360 is as shown in Figure 6.

Figure 6. SalReGCN360 network

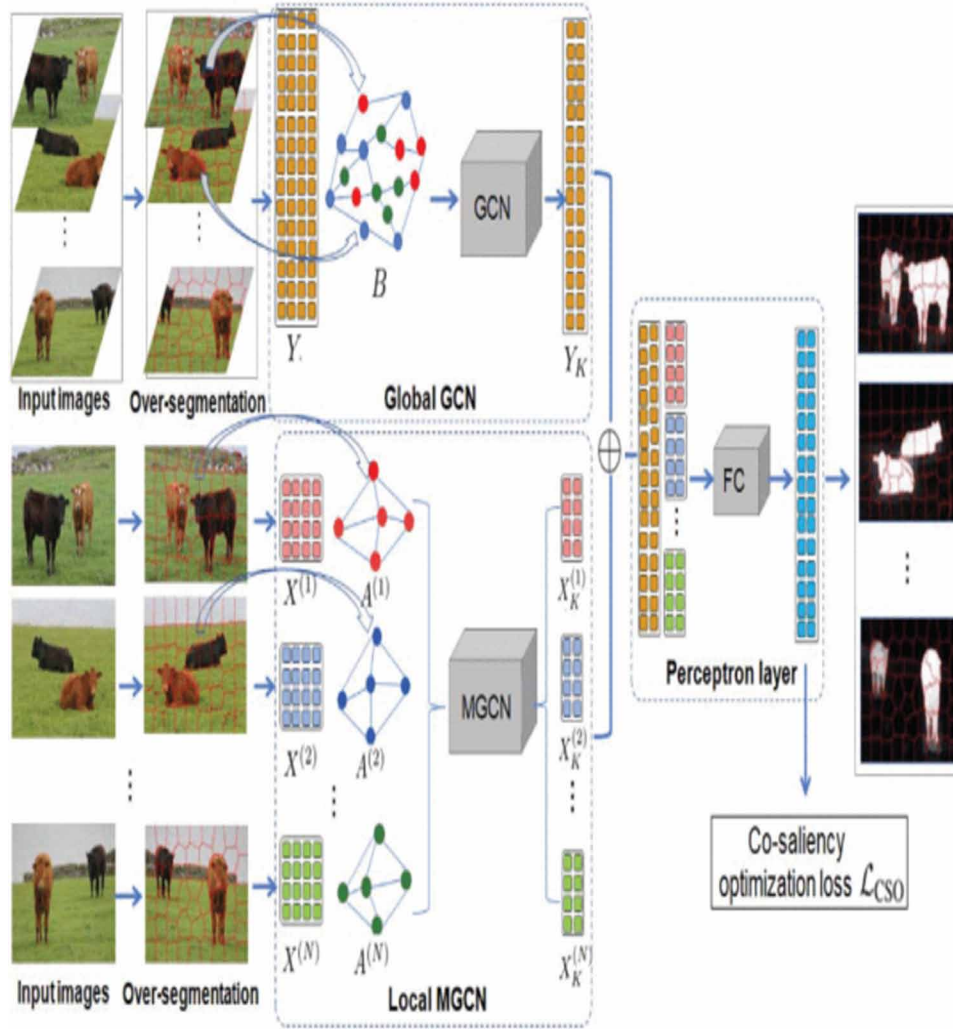
Source: Chen et al. (2022)



For image saliency detection, Geometry Auxiliary Salient Object Detection for Light Fields via Graph Neural Networks, (Zhang et al., 2021) introduced a light field salient object detection approach that leverages graph neural networks to examine the geometric correlations between angular views and central view. The spatial and disparity links between angular and central views are fully mined using a multi-scale graph neural network. A multiscale saliency feature consistency learning module is also recommended in this technique to train clusters of saliency features with good consistency. Figure 7 illustrates the approach's design.

In the research (Ji et al., 2019), a brand-new neural network for detecting saliency is suggested. A multi-layer graph structure and color property are initially used to estimate an approximation of the position and size of notable things in a photograph. Second, a technique is proposed to enhance the saliency detection results by combining Region Net and Local-Global Net. The recommended method may separate the prominent item with a smooth boundary in complex sceneries and cut down on background noise. It effectively captures salient structural and color information of objects by learning both high-level semantic context and low-level characteristic information. The architecture is as shown in Figure 8.

Figure 7. The architecture for geometry auxiliary SOD for light fields via GNN  
 Source: Zhang et al. (2021)



## AN OVERVIEW OF COMPUTATIONAL MODELS

The Computational Models in GNN and its classification are provided by Zhou et al. (2020) with the categorization of spectral based and spatial based models, propagation modules, sampling and pooling modules, and is as shown in Figure 9.



## Study and Analysis of Visual Saliency Applications

Figure 8. The RLG network

Source: Ji et al. (2019)

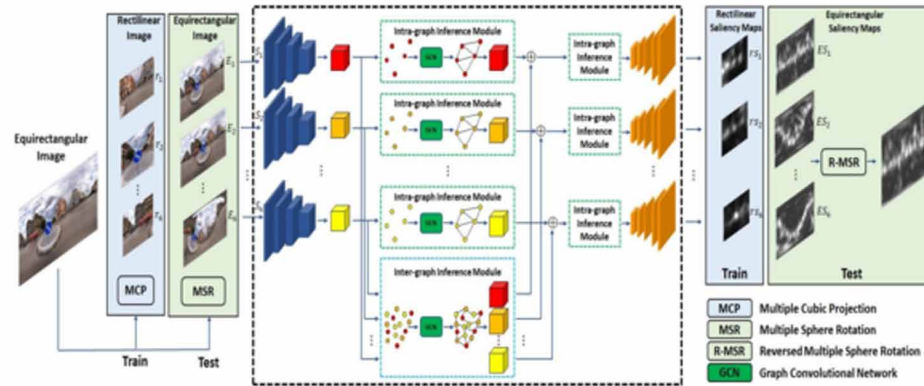
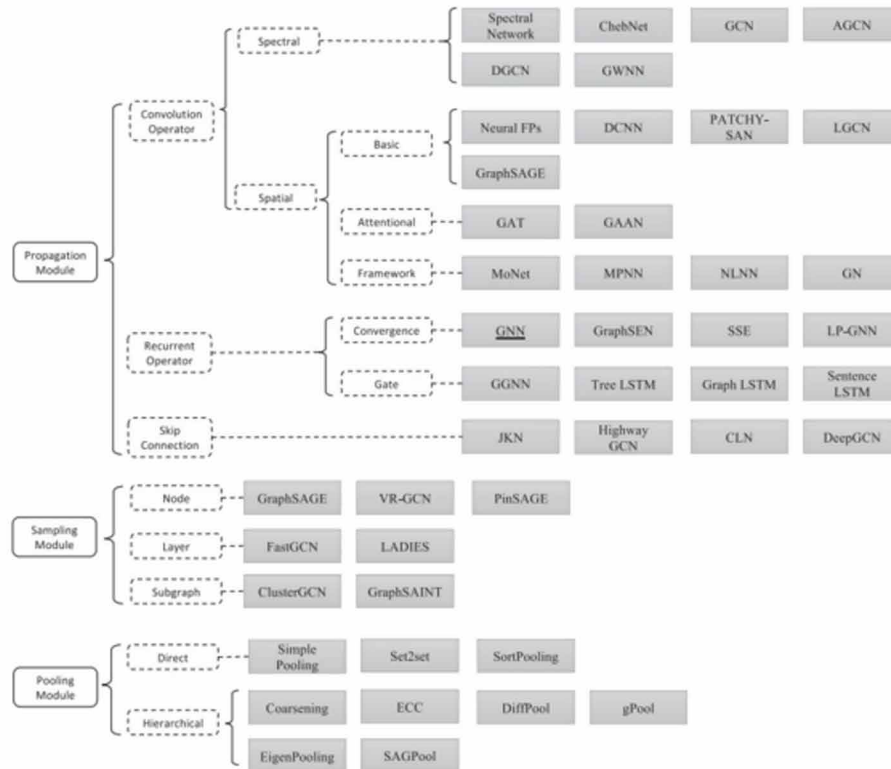


Figure 9. Computational models in GNN

Source: Zhou et al. (2020)



## DATASETS AND EVALUATION METRICS

The popular datasets used for the detection of saliency and co-saliency are summarized in Table 1.

*Table 1. Popular datasets used for saliency and co-saliency detection*

#	Dataset	Year	Images #	Annotation	SOD/Co-SOD
1	MSRA-B	2017	5000	Pixel-wise	SOD
2	DUTS	2017	15572	Pixel-wise	SOD
3	ECSSD	2013	1000	Pixel-wise	SOD
4	DUT-OMRON	2013	5168	Pixel-wise, Eye-fixations, Bounding box	SOD
5	THUS10k	2015	10000	Pixel-wise	SOD
6	iCoseg	2010	643 Images - 38 groups	Pixel-wise	Co-SOD
7	Cosal2015	2015	2015 Images - 58 groups	Pixel-wise	Co-SOD
8	MSRC	2005	240 Images - 7 groups	Pixel-wise	Co-SOD
9	CoCA	2020	1297 Images - 80 groups	Class-level, bounding-box level, object and instance level	Co-SOD
10	CoSOD3k	2021	3000 Images - 160 groups	Hierarchical	Co-SOD

The performance metrics used for salient object detection and co-saliency detection are: Precision-Recall (PR) curve, the Receiver Operating Characteristics (ROC) curve, the average precision (AP) score, and the F-measure, Area Under Curve (AUC), Mean Absolute Error (MAE) (Jiang et al., 2019a). The Evaluation toolbox <https://dpfan.net/CoSOD3K> and <https://github.com/zzhanghub/eval-co-sod.git> repository might be helpful in the calculation of performance metrics of co-saliency methods. [https://github.com/zyjwuyan/SOD\\_Evaluation\\_Metrics.git](https://github.com/zyjwuyan/SOD_Evaluation_Metrics.git) is one of the publicly available repositories for calculating the performance metrics of SOD methods.

## RECOMMENDATIONS

In the work a comparison between RNN and GNN (Di Massa et al., 2006), the results of the approach that use GNNs outperforms RNNs in terms of accuracy with equal error rates for a real-world image classification task.



The SRG approach given in (Tang et al., 2022) outperforms 9 SOTA co-saliency approaches (1-traditional, 8- deep-based methods) and 5 SOD methods as shown in Figure 10. The relationships in most of the graph-based Co-SOD algorithms are represented by scalars in adjacency matrices, which are insufficient for modelling the complex context information in co-saliency detection and are also inapplicable to the DRL (Deep Reinforcement Learning) framework. So, each relationship in SRG is represented as a learnable vector, which can improve node interactions and support the modelling of robust structural semantic relationships by DRL (Tang et al., 2022).

From the previous evaluation, it is observed that the Graph Convolutional Network when combined with a learning factor have achieved competitive results in co-saliency object detection. The Graph neural networks will have a promising future in many computer vision problems, especially SOD and other models may be discovered in the future.

## **CHALLENGES WITH GNN**

Despite the substantial success that GNNs have had in several domains, it is surprising that GNN models are not sufficient to provide satisfactory answers for each graph under any situation. However, there are a number of issues that ought to be resolved in the future.

### **Robustness**

GNNs are a class of models based on neural networks that are subject to adverse assaults. Attacks on graphs take into consideration about structural information than adversarial attacks on images or text, which simply concentrate on features. Several works have been proposed to attack existing graph models (Zugner et al., 2018; Dai et al., 2018) and more robust models are proposed to defend (Zhu et al., 2019).

### **Interpretability**

Applying GNN models to practical applications with reliable justifications is crucial. Few methods (Ying et al., 2019; Baldassarre & Azizpour, 2019) suggested example—level explanations. The area of interpretability on graphs is a crucial one to research, much like the disciplines of CV and NLP.

### **Graph Pretraining**

Neural network-based models need a lot of labelled data, but getting a lot of large-scale human-labeled data is expensive. To help models learn from unlabeled data that is accessible through websites or knowledge bases, self-supervised approaches are presented. With the concept of pretraining, these techniques have had considerable success in the fields of CV and NLP (Bao2021). Pretraining on graphs has been the subject of recent research (Zhang et al., 2020a), however they each have a distinct issue setting and emphasize a different topic.

There are still a lot of unsolved issues in this area that want more study, such as how pretraining tasks should be created, how well-suited present GNN models are for learning structural or feature information, etc.

## CONCLUSION

In machine learning and other related fields, graph convolutional network models, one subset of graph neural network models, have gained a lot of attention. Several models have been suggested to address various applications. In this chapter, we have outlined about the basics of GNN, motivation towards GNN, and its importance in the branch of salient object detection. The strategies employed in the salient object identification field are part of this chapter. Feature-based models, deep learning-based approaches, and graph-based models are among these methods. With the emergence of advanced object detectors, the prominent object detection application has steadily expanded into a wide range of industries, including transportation, agriculture, medicine, and remote sensing. The research currently conducted in the domains of SOD and Co-SOD were reviewed. Further, the use of GNN in salient object detection, GNN models and implementation challenges are also summarized. The authors of this chapter hope that the chapter will help the readers to understand the basics of visual saliency, importance of visual attention, salient object detection methods based on feature, deep, and GNN. The different research approaches that used GNN to find Co-saliency between objects are also incorporated. The challenges of GNN will show a scope for future research.

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## KEY TERMS AND DEFINITIONS

**Attention:** A mechanism that allows a neural network to focus on specific parts of an input.

**Bottom-Up Saliency:** Saliency that is driven by low-level features of the input, such as color, brightness, and orientation.

**Co-Saliency:** A property of multiple images that makes them share common salient objects or regions.

**Co-Saliency Dataset:** A collection of multiple images that share common salient objects or regions, used for training and evaluation of co-saliency models.

**Co-Saliency Detection:** A process of detecting and segmenting common salient objects or regions in multiple images.

**Co-Saliency Integration:** A technique for integrating co-saliency information with other computer vision tasks, such as object recognition and segmentation.

**Co-Saliency Map:** A map that represents the degree of co-saliency of each location or region in multiple images.

**Co-Saliency Pooling:** A technique for aggregating information from multiple images to generate a co-saliency map.

**Edge:** A representation of the relationship between two nodes in a graph.

**Fixation:** A period of time during which the eyes are fixated on a specific location in the visual field.

**Graph:** A data structure that represents objects (nodes) and their relationships (edges).

**Graph Convolutional Network (GCN):** A type of GNN that uses convolutional layers to learn features of the nodes in a graph.

**Graph Neural Network (GNN):** A type of neural network designed to work with graph data structures, where the nodes and edges in a graph are used as input and output.

**Message Passing:** A process by which information is passed between nodes in a graph.

### ***Study and Analysis of Visual Saliency Applications***

**Node/Vertex:** A representation of an object in a graph.

**Saliency:** A property of visual stimuli that makes them stand out from their surroundings and attract attention.

**Saliency Map:** A map that represents the degree of saliency of each location or region in an image or video.

**Top-Down Saliency:** Saliency that is driven by high-level factors such as task demands and prior knowledge.

**Visual Attention:** A type of attention that focuses on specific parts of an image or video.

**Visual Saliency:** The degree to which a specific location or region in an image or video stands out and attracts attention.

## Chapter 9

# Application and Some Fundamental Study of GNN In Forecasting

**Arun Kumar Garov**

*Lovely Professional University, India*

**Ram Kumar**

*Lovely Professional University, India*

**A. K. Awasthi**

*Lovely Professional University, India*

**Monica Sankat**

*Lovely Professional University, India*

### ABSTRACT

*The chapter consists of the application of GNN with all applied fundamentals in different fields of application. Firstly, the discussion will be about the graph using graph theory connection to the mathematical aspect. Secondly, the basis of the data set will be for forecasting and predictive analysis, application, and fundamental concepts, which will help in decision making regarding the different unsolved problems. Third, knowledge about the models of the graph neural network with the examples will be a very important part of the chapter. This chapter is useful for fulfilling the research gap in the field of some forecasting models using graph neural networks with the application of machine learning on data analysis with a large number of examples.*

### INTRODUCTION

This chapter discussed the application of the neural network, such as Graph Neural Networks (GNN). Which is used in the process of the graph, but it is not the only application for the process of the graph of Neural Networks. Two types of neural network applications apply for the process of the graph as; Graph Neural Networks and Recursive Neural Networks. So, Graph Neural Networks is the process of the graph it is clear from the above lines, before see, some ideal knowledge of graph, neural network and then come on to the main point of Graph neural network and application of Graph neural network, understand by examples and case study, etc.

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## GRAPH

A graph is a binary relation to a set of objects. Graphs arose as diagrams representing specific relations among a set of objects. They have the great expressive power to describe the complex relationship among data objects. They can be used to model situations that occur within certain kinds of problems. Such as; In computer science, graphs are used to represent networks for communication, computational devices, etc.

*“Graphs are everywhere.”*

A graph is a type of data structure made up of vertices and edges. It serves as a mathematical framework for examining the relationships between objects and entities pairwise. A graph is typically defined as  $G = (V, E)$ , where  $V$  is a collection of nodes and  $E$  denotes the connections between them.

**Definition (Undirected Graph).** Let  $G$  be an undirected graph,  $G = (V, E, A)$ ,  $V$  is a set of  $m$  vertices, as  $V = \{1, 2, 3, \dots, m\}$ ,  $S \subseteq V \times V$  is the set of edges and  $A \in \mathbb{R}^{m \times m \times k}$  contains the node and edge features with its diagonal components  $A_{i,i,u}$  denoting node attributes and off-diagonal components  $A_{i,j,u}$  denoting edge attributes. Adjacency matrix,  $A \in \{0, 1\}^{m \times m}$  of  $G$  with  $A_{i,j}$  equal to one, iff  $(i, j) \in S$ . let's suppose there is no given node or edge feature, then use  $A = A$ . Otherwise,  $A$  can be considered as the first part of  $A$ , i.e.,  $A = A_{u,u,1}$ . Graph Laplacian denoted by  $L$  and defined as,  $L = A_{i,i,u} - A$ .

Basically, two types of graphs an undirect graph and a direct graph, see Figure 1. And some other kinds of graphs are null graph, connected graph, regular graph, cyclic graph, acyclic graph, Trivial graph, Simple graph, dis-connected graph, complete graph, bipartite graph, complete bipartite graph, star graph, weighted graph, multi-graph, planar and non-planar graph.

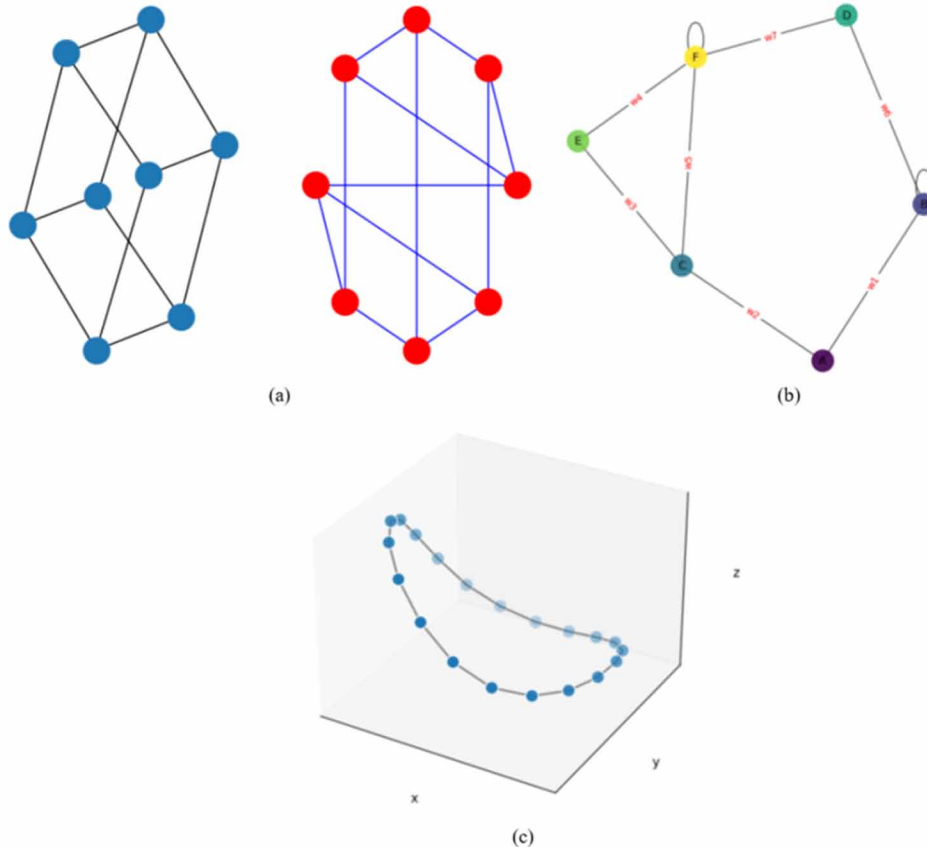
Figure 1. Graph of un-direct and direct



Figure 2 shows different types of graphs plotted by use of jupyter notebook (python 3). Useful command in jupyter notebook as:

In discrete mathematics, study of the graph is known as Graph Theory. Mathematical structure of the connection of points by lines, which is represented into the form of graph. or vertices (nodes), which is connected with the edges (lines). Graph theory not only used in mathematics but also in computer science, physics, chemistry, linguistics, electrical engineering, computer network, social science, biology, etc.

Figure 2. Different graphs plotted in jupyter notebook: a) cubical graph in a different color, b) graph with the edges and labels, c) 3D graph plotted



## Why Is It Hard to Interpret a Graph?

First of all, a graph cannot be represented by any coordinate system we are acquainted with since it does not exist in Euclidean space. As a result, interpreting graph data is far more difficult than interpreting other sorts of data, such as waves, pictures, or time-series signals (including text), which can easily be mapped into 2-D or 3-D Euclidean space. Secondly, a graph does not have a fixed form.

## Why Is Graph Analysis Difficult?

Before creating graph-based solutions, data scientists must be aware of the limitations of graph-based data structures.

1. In non-Euclidean space, there is a graph. It is not present in either 2D or 3D space, making data interpretation more challenging. You need to utilise a variety of dimensionality reduction technologies in order to see the structure in 2D space.

2. Graphs don't have a set form; these are dynamic. Even though two graphs may appear visually dissimilar, these might have comparable adjacency matrix explained. These make it challenging for everyone to do typical statistical analyses of the data.
3. The complexity of the graph for human interpretation will rise with increased size and dimensionality. It is more difficult to comprehend and analyse a complex structure with numerous nodes and thousands of edges.

## **GRAPH-BASED DEEP LEARNING**

Research on this tells the graph roots started from the 1990s era for tree-structured data and neural networks to form recursive neural networks. Later, the RecNN method was rediscovered in relation to applications for natural language processing. It was first used for directed acyclic graph and has since been generalised to many intricate and varied forms.

Due to the interdependencies that exist among the variables described in the neural recursive units, processing cycles posed the major challenge in applying such techniques to generic graphs (acyclic or cyclic, undirected or directed). The Neural Network and the Graph Neural Network for Graphs were the first models to attempt to address this issue.

Similar to the RecNN, the GNN model is built on a state transition system but it allows for cycles in state computation. In order to break the cyclical dependencies in the graph loops with a multi-layered design, the neural network for Graph is based on the premise that mutual dependencies may be controlled by using the representations from earlier levels in the architecture.

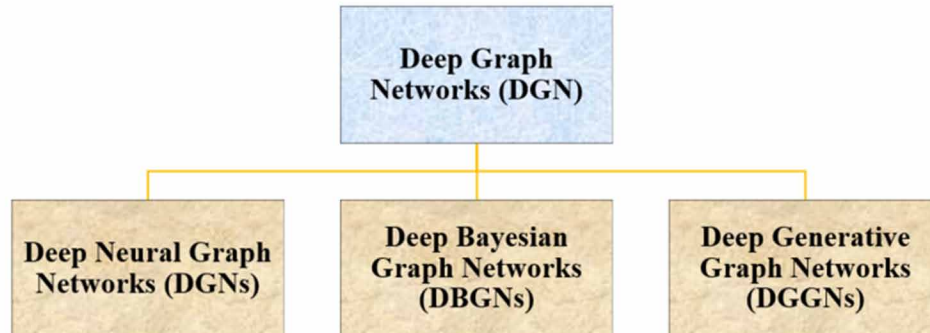
By laying the groundwork for two of the primary techniques for graph processing - the recurrent approaches represented by GNN and the feedforward approaches represented by neural network for Graph-these models have pioneered the area. Under the guise of graph convolutional neural networks, the latter in particular has lately taken the lead.

## **Representation Learning in Graphs**

A portion of the architecture that generates the final internal node representations is referred to as Deep Graph Networks (DGN). These can be attained in one of two ways: by linking all the internal representations calculated at each layer or by taking the internal representations created at the very last layer. A predictor that completes a job by utilising the final internal node representations as input can be paired with any DGN.

DGNs can classify into three main groups: 1). Deep Neural Graph Networks (DGNs), 2). Deep Bayesian Graph Networks (DBGNs), and 3). Deep Generative Graph Networks (DGGNs). Deep Neural Graph Networks (DGNs), in this include model based on neural architectures, Deep Bayesian Graph Networks (DBGNs), which represent probabilistic models of graphs, and Deep Generative Graph Networks (DGGNs), which include generative approaches to graphs that can make use of neural and probabilistic both models.

*Figure 3. Types of deep graph networks (DGN)*



## Modern Deep Learning Architectures for Graph

The types of representations a model may calculate are often determined by the key elements of local graph learning models. Therefore, the research studies describe some of the fundamental components typical of such designs and investigate how they might be put together or integrated to form an efficient learning model for graphs.

The foundation of local graph processing is how models combine neighbours to produce hidden node representations. In accordance with the standard neighbourhood aggregation strategy, arcs must be unattributed or contain the same data. This is not always the case as arcs in a graph frequently carry extra information about the type of link. As a result, procedures that make use of arc labels to enhance node representations are required.

Attention mechanisms, which provide a relevant value to each component of a brain layer's input, are one method that has gained favour, particularly in language-related tasks. Consideration of the aggregation function may be used, when the input is the structured graph, and this produces a weighted average form for the average of the neighbours where individual weights are a function of a node and its neighbour.

Aggregations over all neighbours for each node, however, may not be practical in big, dense networks. To lessen the computing load, alternate methodologies like neighbourhood sampling are therefore required.

## Graph Embedding

With fully connected layers, convolutional layers, pooling layers, etc., graph neural networks can be built much like any other neural network. Depending on the complexity and kind of the graph's data as well as the desired result, the type and number of layers will vary.

The structured graph data is sent into the GNN, which outputs a vector of numerical values that indicate pertinent data about the nodes and their connections.

A term for the representation of vector is known as "Graph embedding". where embeddings are frequently employed to convert complex data into a structure in machine learning that can be recognized and understood. Natural language processing systems use embeddings word to generate numerical representations of words and their relationships.



## How Does the GNN Procreate the Embedded Graph?

The features of each node are joined to those of its nearby nodes when the data of the graph is transferred to the GNN. We refer to this as “message passing.” If the GNN has more than one layer, the message-passing action is repeated by succeeding layers, collecting data.

When applied graph-based deep learning methods in different fields they face some challenges, so here can see for medical diagnostics in the next session.

## Some Challenges in Medical Diagnostic Analysis to Adopting Graph-Based Deep Learning Methods

List the following seven key obstacles to the adoption of graph-based deep learning:

1. Estimation and graph representation
2. Dynamism and temporal graphs
3. The complexity of graph models and the effectiveness of training
4. Clarity of explanation and interpretability
5. Graph model generalisation
6. Effective data annotation and training paradigms
7. Quantification of uncertainty

## INTRODUCTION OF GNN

Strongly structured data may only be processed in certain application domains where topological information representing relationships between various data components must be taken into account. GNN has been modeled to process data represented in graph domains considering the topology of the graph. GNN can handle a broader class of graphs, such as cyclic, directed, and undirected graphs, it is seen as an extension of RNN. The goal of a GNN is to solve a problem by using the encodings that are stored in the states to decode the graph-structured data using the topological relationship between the graph's nodes. The GNN could be learned from instances; consider a function  $\tau$  and  $G$  graph, where function mapping on the graph and  $n$  is one of its nodes to a vector of reals:  $\tau(G, n) \in R^k$ .

Neural Network is a tool used to solve a problem intelligently. Graph neural networks and recursive neural networks are two connectionist models that can handle graphs directly. Although RNNs and GNNs use a similar processing foundation, they may be used with various input domains. RNNs need directed and acyclic input graphs, but GNNs can handle any type of graph.

Due to its utility and simplicity in the domains of pattern recognition and data mining, neural networks have greatly increased in popularity in recent years. The usage of CNN, RNN, and autoencoders in Deep Learning for tasks like object identification and speech recognition have led to a significant investment in the research and development of neural networks.

Which are based on Euclidean network data sets, deep learning may be used to quickly analyse things like images, text, and videos. likewise, also crucial to consider situations where data is shown in complex non-Euclidean networks with sophisticated connections between items. for that use, a Graph

Neural Networks comes into play (GNN). This chapter will discuss a few of the current applications of Graph Neural Networks as well as the concepts and principles of Graphs and GNNs.

## Mathematical Concept of Graph Neural Network

**Definition (GNN):** A GNN is an invariant function mapping from the space of  $(S, \mathbf{A})$  to  $\mathbb{R}^d$ . More specifically, a GNN first performs multiple invariant message passing operations to compute a node embedding  $z_i = GNN(x, \mathbf{A})$  for all  $x \in S$ , and then performs a set aggregation (pooling) over  $\{z_i | i \in S\}$ , describe as  $AGG(\{z_x | x \in S\})$ , as the set  $S$  represent by  $GNN(S, \mathbf{A})$ .

Let  $G$  be a graph as  $G = (V, E)$ ,  $V$  represents a set of vertices called nodes, and  $E$  is a collection of edges linking two nodes of  $V$ . Let  $ne[m]$  be the set of all nodes connected to the node  $n$  by arcs in  $E$ . The nodes of  $G$  are attached with labels  $l_m \in R^c$  and the edges with label  $l_e \in R^d$ . In Graph Neural Network a state vector  $x_m \in R^s$ , which represents the characteristics of the node (i.e., adjacent nodes, label, degree, etc.), is attached to each node  $n$ . The state vector of a node with dimension  $s$  is computed using two feedforward neural networks, transition network and forcing network, which implement a local transition function  $f_w$  (Baskararaja et al., 2012; Roy et al., 2021).

$$\begin{aligned} x_m &= f_w(l_m, x_{ne[m]}, l_{ne[m]}) \\ &= \sum_{v \in ne[m]} h_w(l_m, x_v, l_v) \end{aligned}$$

$h_w$  is a function of the state, the label of the neighbouring node, and its own label for each of the  $m$  nodes. The neighbours of the transition network determine how many input patterns it has. Considered that  $h_w$  is a linear function.

$$h_w(l_m, x_v, l_v) = B_{m,v} x_v + A_m$$

where  $A_m \in R^s$  is defined as the output of forcing network which implements  $\rho_w : R^c \rightarrow R^s$ , that is

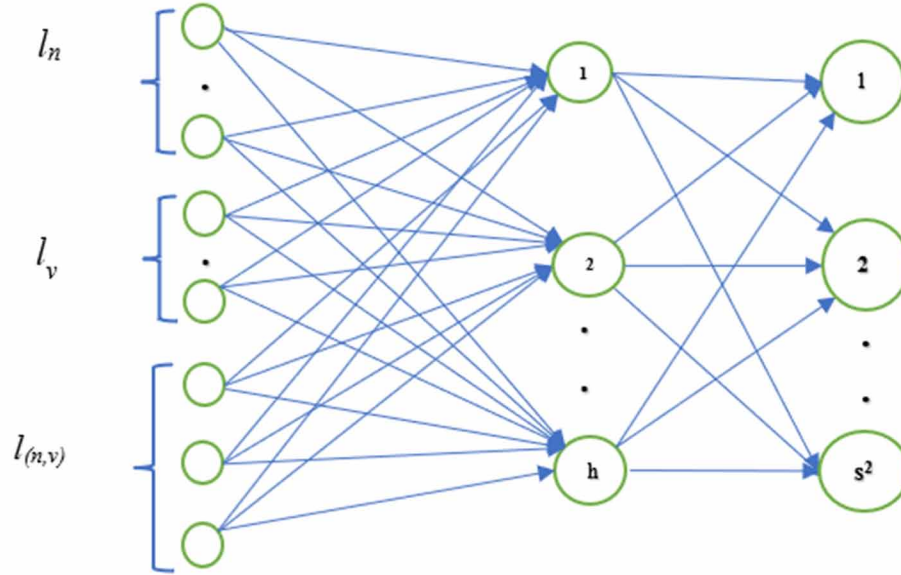
$$b_m = \rho_w(l_m).$$

$B_{m,v} \in R_{s \times s}$  is defined as the output of the feedforward neural network called transition network which implements  $\phi : R^{2c+d} \rightarrow R^{s^2}$ .

$$B_{m,v} = \frac{\mu}{s \times |ne[m]|} \text{resize}(\phi_w(l_m, x_v, l_v)) \mu$$

where  $\mu \in (0, 1)$  and  $\text{resize}$  operator arranges  $s^2$  elements of the output of transition network into a  $s \times s$  matrix. Figure 4 represents the transition network of a node  $n$  with label  $l_n$  of a graph.

Figure 4. Transition network on  $n$  nodes



Let's denote the vector created by stacking all of the states and labels of the graph  $Y$ ,  $l$ . Then, it is possible to write,

$$Y = F_w(Y, l)$$

where the global transition function is called  $F_w$ . In the iterative approach for computing the state, the Banach fixed point theorem ensures the existence and uniqueness of the solution.

$$Y(t+1) = F_w(Y(t), l)$$

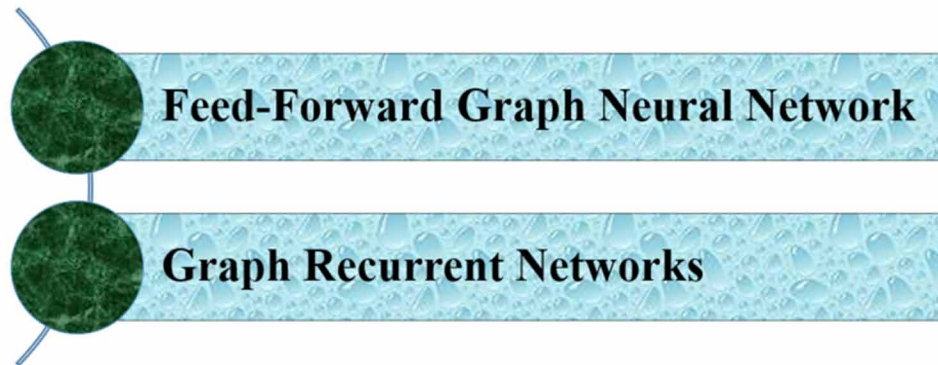
## Architecture of GNN

Two main architectures of GNN (i.e., feed-forward graph neural network and graph recurrent networks).

Applying the transfer function at the edge weights between each node, a feed-forward graph neural network propagates input data across a graph of neurons to produce output.

Similar to feed-forward graphs, which only allow data to flow in one direction, graph recurrent networks also have a graph structure. However, unlike feed-forward graphs, which only allow data to flow in one direction, this graph network graph allows data to flow in both directions.

*Figure 5. Architectures of GNN*



## **Advantages of GNN**

Graph neural networks provide assistance with problems that conventional neural networks haven't yet been able to resolve successfully. A graph's data could not be processed properly because the links between the data were not given enough weight. However, with GNNs, the so-called edges are as significant to the nodes themselves.

## **Graph Neural Networks' Drawbacks (Disadvantages)**

The use of GNNs has some disadvantages. When to utilise GNNs and how to enhance the performance of our machine learning models will both be determined by our ability to comprehend them.

1. In contrast to GNNs, which are shallow networks typically with three layers, most neural networks can go deep to provide higher performance. It prevents us from delivering cutting-edge performance on huge datasets.
2. Since the graph structures are dynamic, it is more difficult to train a model on it.
3. Due to the high computational cost of these networks, scaling the model for production presents challenges. It will be challenging for you to grow the GNNs in production if your graph structure is huge and complex.
4. However, graph neural networks cannot address other issues that arise with neural networks. Particularly, the black box issue has yet to be resolved. The underlying operations of the complicated algorithms are hard to follow from the outside, making it challenging to grasp how a (graph) neural network reaches its ultimate conclusion.

## **Why Are Graph Neural Networks Necessary?**

The study of pattern recognition and data mining has been advanced by recent developments in neural network technology. End-to-end deep learning models like CNN, RNN, or autoencoders have revived machine learning tasks including object identification, machine translation, and speech recognition. Deep learning may be used to successfully capture hidden patterns in Euclidean data (text, videos, images).

Where data creates from non-Euclidean domains and represented as graphs with complex item interactions and dependencies, in these type of situations Graph Neural Networks (GNN) are useful.

Additionally, GNNs are required to address issues with Node Classification, Link Forecast, and Graph Classification.

## **Graph Neural Network Challenges**

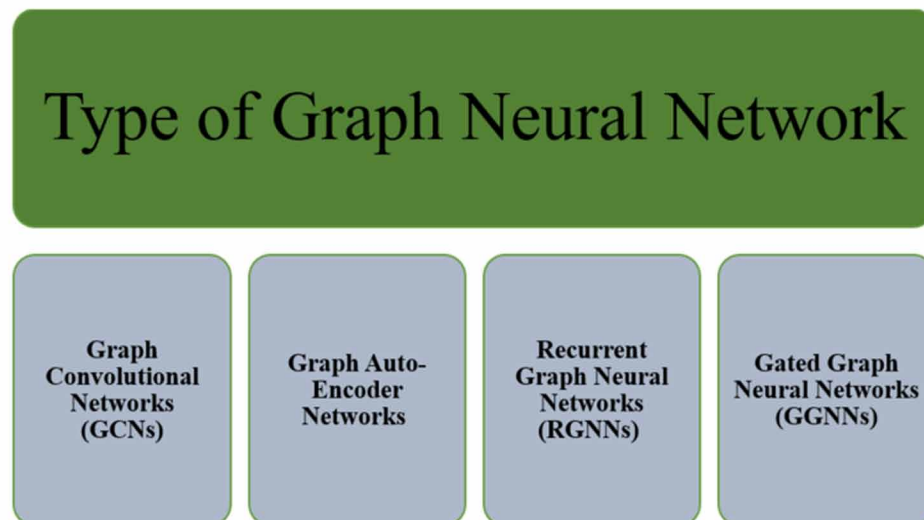
Few challenges of Graph neural network are:

1. **Dynamic Nature:** Since GNNs are dynamic graphs, dealing with graphs with dynamic structures might be difficult.
2. **Scalability:** For all graph embedding techniques, including GNNs, embedding methods in social networks or recommendation systems can be computationally challenging.
3. **Non-Structural Data:** GNN applications in non-structural contexts are likewise challenging. It is difficult to determine the appropriate graph creation method for GNNs.

## **TYPES OF GRAPH NEURAL NETWORK**

This session gives an idea of GNN types:

*Figure 6. Types of graph neural network*



### **Graph Convolutional Networks (GCNs)**

It is comparable to classic CNNs. By looking at nearby nodes, it picks up characteristics. GNNs combine node vectors, send the resulting data to the dense layer, and then use the activation function to

introduce non-linearity. Graph convolution, a linear layer, and a non-learner activation function make up this system, in essence.

Mathematical formulation of GCNs:

$$T_u^v = f^v \left( X^v \frac{\sum_{s \in N_u} T_s^{v-1}}{|N_u|} + C^v T_s^{v-1} \right)$$

Where  $N_u$  represent the neighborhood of node u,  $X^v, C^v$  tells learnable weights and shared among all the nodes, activation function represented by  $f^v$ ,  $T_u^v$  represent node u embedding at step v, v is step, each step corresponding to aggregation information from v-hope neighbors.

User can create a GCN in Python by using PyTorch:

Figure 7. Programming in Python

```
import torch
from torch import nn

class GCN(nn.Module):
    def __init__(self, *sizes):
        super().__init__()
        self.layers = nn.ModuleList([
            nn.Linear(x, y) for x, y in zip(sizes[:-1], sizes[1:])
        ])
    def forward(self, vertices, edges):
        # ----- Build the adjacency matrix -----
        # Start with self-connections
        adj = torch.eye(len(vertices))
        # edges contain connected vertices: [vertex_0, vertex_1]
        adj[edges[:, 0], edges[:, 1]] = 1
        adj[edges[:, 1], edges[:, 0]] = 1

        # ----- Forward data pass -----
        for layer in self.layers:
            vertices = torch.sigmoid(layer(adj @ vertices))

        return vertices
```

Spatial convolutional networks and spectral convolutional networks are the two main forms of GCNs.

## Spatial Convolutional Network

Spatial diagram Convolutional networks use the spatial features of graphs in spatial space to learn from them. The spatial convolution network functions similarly to CNN, which rules the research on segmentation tasks and picture classification.

Convolution, in its simplest form, is the idea of adding neighbouring pixels to a centre pixel, where the neighbouring pixels are chosen by a filter with learnable weight and adjustable size. Spatial convolutional networks, which merge the characteristics of neighbouring nodes into the centre node, use the similar principle.

## **Spectral Convolutional Network**

This type of graph convolution network has significantly deeper mathematical foundations compare to differ type of Graph NN. Spectral Convolutional networks are based on graph signal processing theory. Simplification is also used to mimic graph convolution.

These networks use the eigen-decomposition of the graph's Laplacian matrix in addition to Chebyshev polynomial approximation to spread information along nodes. The way waves propagate over signals and systems served as the inspiration for these networks.

## **Graph Auto-Encoder Networks**

It attempts to rebuild input graphs using a decoder after learning graph representation using an encoder. A bottleneck layer connects the encoder and the decoder. Due to the fact that auto-encoders are effective at handling class balance, they are frequently utilised in link prediction.

## **Recurrent Graph Neural Networks (RGNNs)**

It can handle multi-relational networks where a single node has numerous relations and learns the optimal diffusion pattern. Regularizers are used in this form of graph neural network to improve smoothness and reduce over-parameterization. RGNNs produce superior outcomes while utilising less processing power. In addition to text generation, they are also used for machine translation, speech recognition, video tagging, picture description and text summarising.

Recurrent Graph Neural Networks (RGNNs) are able to learn the ideal diffusion pattern and handle multi-relational graphs where a single node has several relations. In this type of graph neural network, regularizers are used to enhance smoothness and decrease over-parameterization. These use less processing power while producing better results.

RecGNN is based on the Banach Fixed-Point Theorem, which asserts that: Let  $(\mathcal{X}, c)$  be a full metric space and  $\alpha : \mathcal{K} \rightarrow \mathcal{K}$  be a contraction mapping. Then  $\mathcal{M}$  has a unique fixed point  $(k^*)$ , and for each  $k \in \mathcal{K}$ , the sequence  $M_n(k)$  for  $n \rightarrow \infty$  converges to  $(k)$ . This suggests that if apply the mapping  $M$  to  $k$  for  $s$  times,  $k^s$  should be close to  $k^{(s-1)}$ .

$$k^s = M(k^{s-1}), s \in (1, n)$$

RecGNN defines a parameterized function  $f_w$ :

$$x_n = f_w(l_n, l_{co[n]}, x_{ne[n]}, l_{ne[n]})$$

Figure 8. Uses areas of recurrent graph neural networks

Common Use of Recurrent Graph Neural Networks (RGNNs)					
Speech recognition	Text generation	Picture description	Machine translation	Video tagging	Text summarizing

where  $l_n, l_{co}, x_{ne}, l_{ne}$  represents the features of the current node  $[n]$ , the edges of the node  $[n]$ , the state of the neighboring nodes, and the features of the neighboring nodes.

Finally, after  $s$  iterations, the final node state is used to produce an output to make a decision about each node. The output function is defined as:

$$O_n = g_n(x_n, l_n)$$

Let see the Architecture of RGNN in Figure 10.

### Gated Graph Neural Networks (GGNNs)

A gated graph neural network is a popular message-passing layer variant. The final equation, the node update, is changed to

$$\vec{v}_i' = GRU(\vec{v}_i, \vec{e}_i)$$

where the gated recurrent unit is GRU. A GRU is a type of binary neural network with two input arguments that are frequently applied to sequence modelling. The intriguing difference between a GGN and a GCN is that the former contains trainable parameters in the node update (from the GRU), which gives the model a little more latitude. Similar to how a GRU is used to represent sequences, the GGN maintains the same GRU settings at every layer. Being able to build limitless GGN layers without increasing the amount of trainable parameters is a good feature of this (assuming you make  $W$  the same at each layer). GGNs are therefore appropriate for big graphs, like a big protein or a big unit cell.



## Application and Some Fundamental Study of GNN In Forecasting

Figure 9. Graph and the neighborhood of a node. The state  $x_i$  of the node  $i$  depends on the information contained in its neighborhood.

Source: Scarsell et al. (2008)

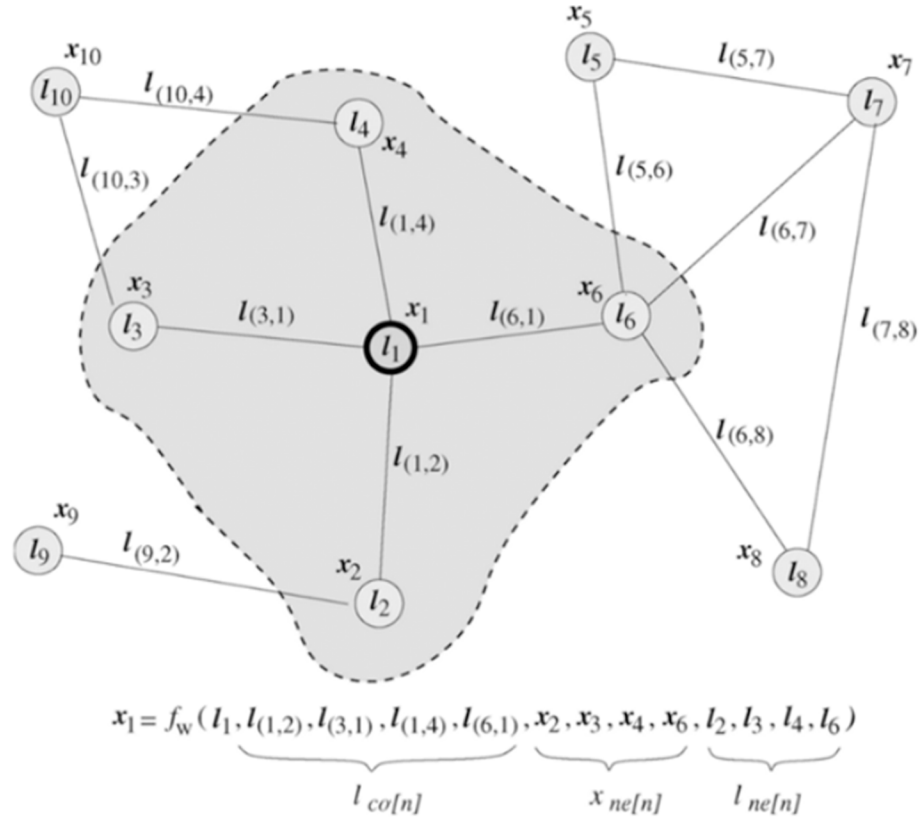
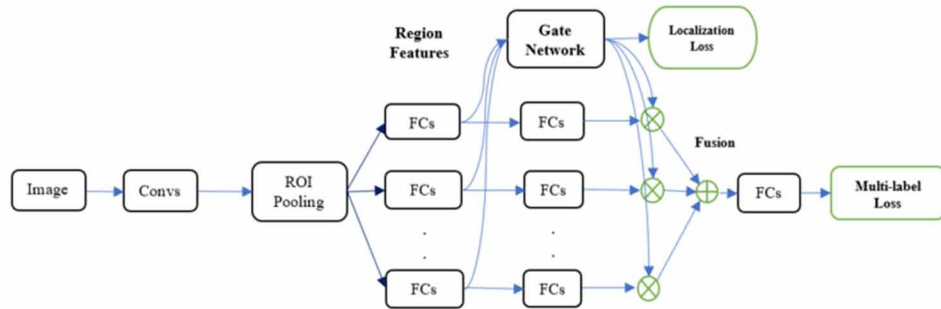


Figure 10. RGNN architecture

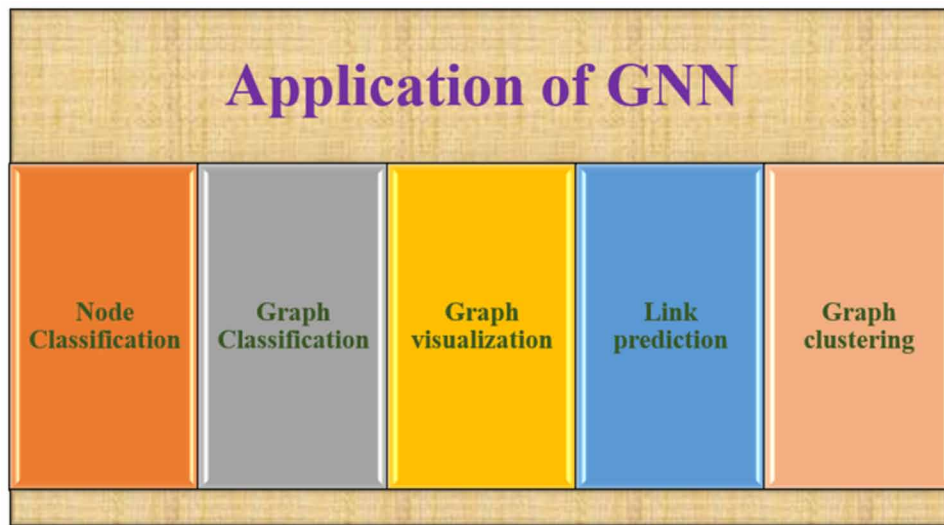


When completing jobs with long-term dependencies, it performs better than RGNN. Recurrent graph neural networks are enhanced by adding nodes, edges, and temporal gates for long-term dependencies in gated graph neural networks. Gates are used to recall and forget information in various stages, much like Gated Recurrent Units (GRU).

## APPLICATIONS OF GNNs

The above has been discussed about the basic idea of the GNN and Graph theory. This session is based on the application of the GNN in some categories, which is shown with a few applications of GNNs. Graph-structured data is present everywhere/every sector. These categories may be used to group the issues that GNNs solve:

*Figure 11. Application of GNN*



**Node Classification:** There involves classifying samples (represented as nodes) by examining the labels of the nodes around neighbors. This kind of issue is often taught semi-supervisedly, with only a portion of the graph labeled.

**Classification of Graphs:** Sorting the entire graph into separate groups is the work at hand in it. The focus shifts to the graph domain, similar to picture categorization. Graph classification has several uses, including detecting whether or not a protein is an enzyme in bioinformatics, classifying articles in natural language processing, and social network analysis.

**Graph Visualization:** Information visualisation and geometric graph theory meet in the field of graph visualisation, a branch of mathematics and computer science. It is concentrated on the visual representation of graphs that aids the user in understanding the graphs by exposing structures and potential anomalies in the data.

**Link Prediction:** In this, the algorithm must comprehend how entities interact in networks and attempt to foretell if two entities are connected. Inferring social relationships or recommending potential buddies to users is crucial in social networks. It has also been used to difficulties with recommender systems and the identification of criminal links.

**Graph Clustering:** Data clustering in the form of graphs is referred to as graph clustering. On graph data, clustering is done in two different ways. By using edge weights or edge distances, vertex clustering attempts to arrange the graph's nodes into highly linked clusters. The second method of clustering graphs does so by treating the graphs as the items to be grouped and grouping them according to similarity.

Various fields applications of the GNN also can be discussed, such as computer vision, traffic, chemistry, natural language processing, etc, which is discussed here;

Let's go over some examples from various fields where GNN may address various problems.

- **Computer Vision Using GNN**

Machines can differentiate and identify objects in pictures and movies using standard CNNs. However, considerable work must be done before robots can exhibit human-like visual intuition. GNN architectures, however, can be used to solve picture categorization issues.

One of these issues is scene graph generation, where the model attempts to separate a picture into an object-and-relationship semantic network. Scene graph generation models can identify things in a picture and foretell the semantic links that exist between them when they are paired.

GNNs are still being used in a rising number of computer vision applications, nevertheless. It also covers things like human-object interaction and few-shot picture categorization.

- **Natural Language Processing With GNNs**

According to NLP, text is a kind of sequential data that may be characterised by an RNN or an LSTM. However, since they are so natural and simple to express, graphs are frequently employed in numerous NLP tasks.

The use of GNNs for several NLP issues, including text categorization, using semantics in machine translation, user geolocation, relation extraction, and question answering, has seen a recent uptick in attention.

Every node is recognised as a separate entity, and edges define the connections between them. The issue of question answering has long existed in NLP research. However, it was constrained by the current database. Although the methodology may be extended to previously undiscovered nodes (as a forecasting) using strategies like GraphSage,.

- **GNNs in Traffic**

The capacity to predict traffic volume, speed, or road density is a crucial element of a smart transportation system. We can resolve the traffic prediction issue using STGNNs.

Think of the traffic network as a spatial-temporal graph, with nodes standing in for the sensors positioned on the roads, edges for the distance between pairs of nodes, and dynamic input characteristics for the average speed of traffic for each node during a window.

- **Chemistry With GNNs**

Chemists can utilise GNNs to investigate the graph structure of molecules or compounds in the field of chemistry. Atoms serve as nodes and chemical bonds serve as edges in these graphs.

- **GNNs in Other Domains**

GNNs can be used for more than only the tasks and domains listed above. Program verification, programme reasoning, electrical health records modelling, brain networks, social influence prediction, recommender systems, and adversarial attack avoidance are just a few of the issues to which GNNs have been attempted to be used.

## **PYTHON LIBRARIES FOR GNN**

Let's explore some open-source libraries in high quality for graph neural network in this session, which is help to use of python for GNN, see Figure 12.

*Figure 12. Useful libraries of Python for GNN*

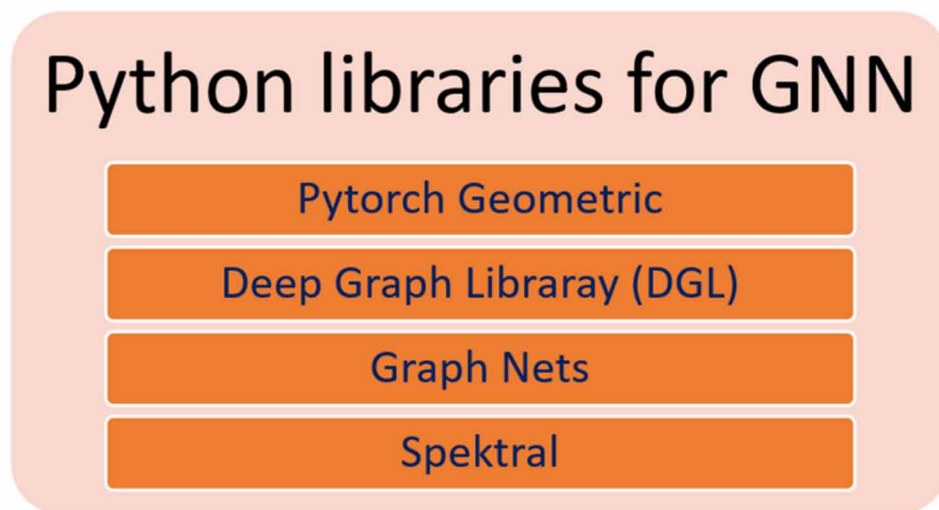


Figure 12 shows the library but which one is best and how to choose.

The user chooses the library that is best suitable for own's needs, and this decision is typically impacted by the deep learning libraries user or user's manager/teammate used in the past. For instance, Spektral may be a nice library for a user if user has experience with or is accustomed to using Keras and Tensorflow. Due to TensorFlow 1, at beginning do not use a new GNN project with the Graph Nets DeepMind library. As well if a user is working on legacy projects, it's a logical decision.

PyTorch Geometric is a solid option if user is looking for a quick, capable library at a reasonably established and mature stage of development, with the ease of integration of standard benchmark datasets to implementation of other publications.

## GRAPH NEURAL NETWORK (GNN) FORECASTING-BASED MODELS

The previous section discussed basic and conceptual knowledge of graph, graph neural network with its applications and with examples. In the next section, we will discuss a case study to understand the forecasting analysis.

### Case Study 1

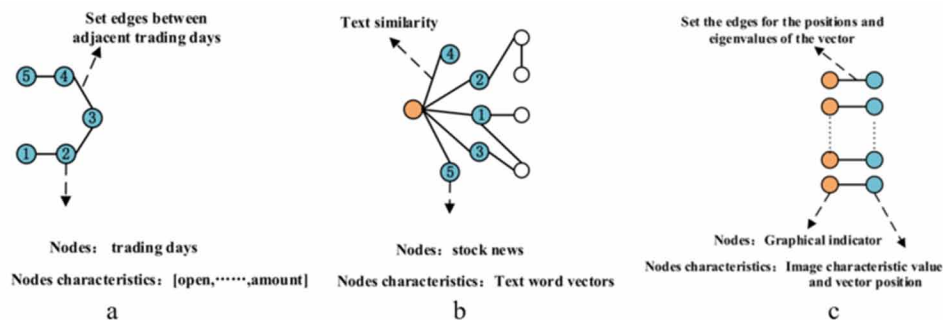
In this case study discussed about the stock market index forecasting, which is based on a graphical neural network. Taken a heterogeneous data as stock market index data, news of stock market, graphical indicators for this process. Build a subgraph of these data, which based on the weighted of edges (Li et al., 2022).

Used stock market index data of Shanghai Composite Index, Shenzhen Composite Index, and China Securities Index (CSI) 300, from 11 Jan 2013 to 25 Nov 2019. Deep Graph Library (Dgl) is used to create graph data and perform the necessary convolution. The news index subgraph builds the connections between news texts by treating each news item as a graph node, using the word vector of the news text as the corresponding node feature, and using the similarity of the news text as the edge weight. The stock market has a subgraph every day. The news texts are transformed into 200-dimensional word vectors as node characteristics using the genism package. A similarity model uses the weights of the news subgraph edges to determine the similarities between news texts. Figures 13 and 14 are the type of stock market indicators and graphical embedding of data.

Figure 13. Data type of stock market indicators



Figure 14. a) Trading subgraph embedding, b) news subgraph embedding, c) graphical indicator subgraph embedding



Six indices-the minimum index, maximum index, opening index, trading volume, closing index, and number of transactions during each trading day-are used as node characteristics in the subplan for the trading data indicators, which chooses five working days as nodes. The starting weight of each subgraph edge is a random number in the range [0, 1], and an edge is established between adjacent trade days. A K plot, a 5-day moving average, and a 20-day moving average are all included in the graphical index subplot. Using the cv2 package, the graphical index picture is spliced into the BGR channel and stitched into a vector. The vector's redundant values of 190, 191, and 51 are removed, and 30,000 values are chosen at random to serve as the training data. The construction of 200 node plots with Three hundred -dimensional features per node. The position values of the graphical index eigenvectors are represented by node features 99–199, whereas node features 0-99 represent the eigenvalues of the graphical index eigenvectors. For the corresponding node, an edge is created. Each edge's starting weight is a random number between [0, 1].

LSTM method used for the performance of node aggregation and train shared weight parameters between the aggregation process.

Used method for the trading of stock market:

1. TeSIA
2. MHDA
3. Msub-GNN

Vertex filtering for stock market news index subgraphs is performed using edge weights, and an attention mechanism based on the edge weights is realised. To update the model parameters, conventional stochastic gradient descent and back propagation techniques are used. According on how closely the compared news texts resemble each other, the starting weight of each edge is determined.

The stock market news graph data edge's weight is adjusted during the model iteration procedure using equation 1. Equation 2 is used to score the edge weights in order to optimise them, allowing the model to produce more precise neighbourhood nodes for vertex embedding (Awasthi et al., 2023).

$$\delta_{ij}^r = \text{soft max}_i(e_{ij}^r) \quad (1)$$

To make the edge weight matrix simple to compute and compare, equation (1) regularises the edge weight matrix  $e_{ij}^r$  to produce the regularised edge weight matrix  $\delta_{ij}^r$ .

$$e_{ij}^r = \text{Leaky ReLU} \left( \vec{a}^T \left[ Wh_i \parallel Wh_j \right] \right) \quad (2)$$

Edge weights choose the neighbourhood nodes, which are embedded vertices. Out of the five linked nodes, N notifies the node with the highest edge weight. Applying equations 3,4, and 5 yields the embedding procedure for the vertex characteristics of the neighbourhood nodes.

$$h_{yN(i)}^{t+1} = \text{LSTM} \left( \{h_{yj}^t, \forall j \in N(i)\} \right) \quad (3)$$

$$h_{yi}^{t+1} = \sigma \left( wconcat \left( h_{yj}^t, h_{yN(i)}^{t+1} \right) \right) \quad (4)$$

$$h_{yi}^{t+1} = norm \left( h_{yi}^{t+1} \right) \quad (5)$$

After the subgraph convolutions are aggregated, the updated information  $m_{mi}^t$  is eventually retrieved via the node hidden states  $h_{xi}^{t+1}$ ,  $h_{ki}^{t+1}$ , and  $h_{di}^{t+1}$  and the three-dimensional tensor  $A_{aij}$  utilised to carry out message transmission  $m_{mi}^t$ . The three types of edge connection subgraphs, building up a three-dimensional tensor of edge weights  $A_{aij}$  to represent the degrees of correlation among different index.

$$\beta_{\phi_i} = \frac{\exp(m_{\phi_i})}{\sum_{i=1}^P \exp(m_{\phi_i})} \quad (6)$$

The weight coefficient illustrates how crucial the metapath is for categorising and forecasting the intricate network of the stock market. And,

$$m_{\phi_i} = \frac{1}{|V|} \sum_{i \in V} a^T \cdot \tanh \left( A_{aij} \cdot h_{mi}^{\phi_i} + h \right)$$

Where,  $m_{\phi_i}$  is metapath.

The final aggregate node (N) employs two different attention techniques based on the traditional characteristics of nodes. Semantic layer and the node layer are created to hold significant information.

$$N = \sum_{i=1}^P \beta_{\phi_i} N_{\phi_i}$$

Where  $\phi_i$  is a different metapath weight coefficient and  $N_{\phi_i}$  is node-level attention mechanisms.

TeSIA combines data from several sources to provide a baseline for forecasting, and it has been successful in a number of multi-source data forecasting applications. There is no data verification phase based on the vector approach since this method is based on the tensor data processing method. Figure 15 shows the comparison of the used method benefits.

In order to anticipate stock market trends, this case study demonstrates the use of a graph neural network for the fusing of multi-source heterogeneous subgraphs. This new network constructed a trade data index subgraph, a stock market news index subgraph, and graphical indicators in addition of types of embedded representation techniques for stock market indexes. This network employed several convolution techniques to aggregate node pair data in graphs.

In this case study, a strategy that accomplishes semantic data mining and expressed the correlation relationships among the forecast indices are used, successfully increasing the stock market trend forecasting's accuracy.

Figure 15. Comparison of used method benefits

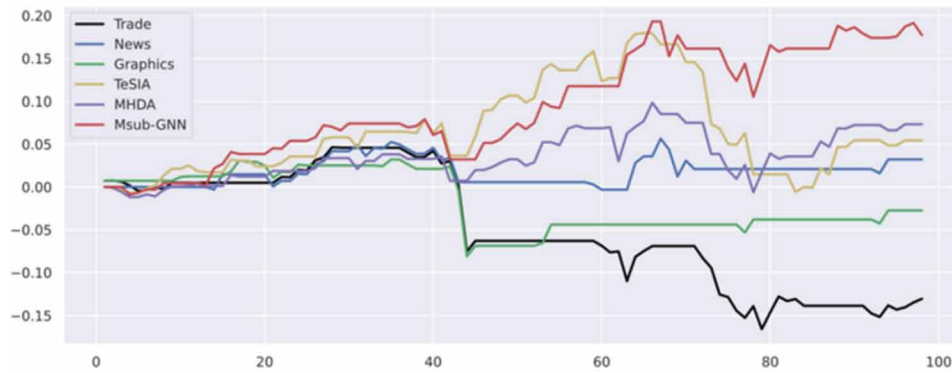


Table 1.

Methods	Information_Ratio	Sharpe_Ratio	Sortino_Ratio	Max_Drawdown
News	0.346	0.416	0.534	33.58%
Trade	0.372	0.437	0.562	38.29%
Graphics	0.426	0.451	0.685	36.28%
TeSIA	1.132	0.847	1.126	28.71%
MHDA	1.332	0.876	1.116	30.12%
Msub-GNN	1.413	0.978	1.325	21.53%

## Case Study 2

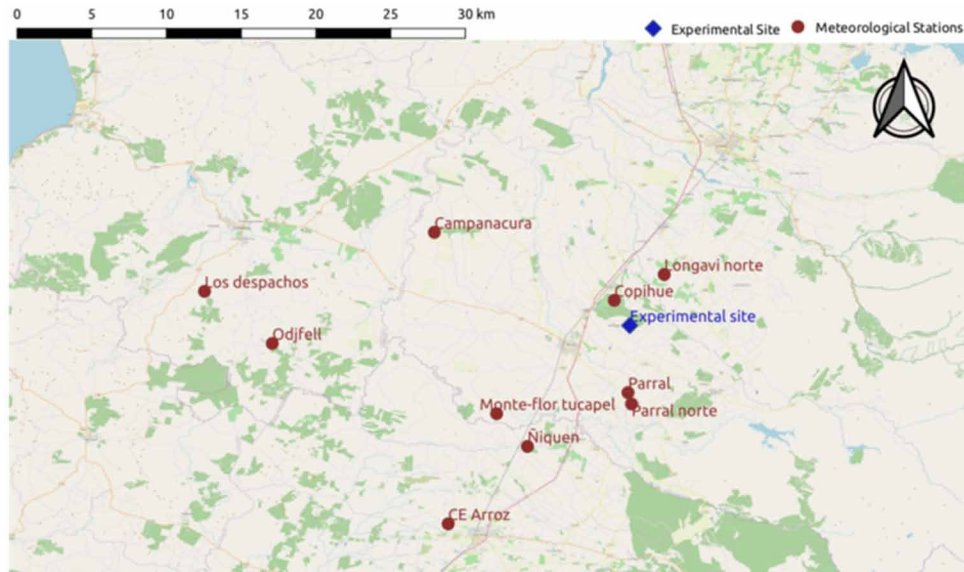
This case study is based on the GSTA\_RRC model's forecasting of the minimal temperature for a set number of hours in the future in a local experimental area (Lira et al., 2021).

Data from air temperature and air humidity sensors set at a nearby orchard of Chilean are used in this case study. Twelve low-power wireless modules-eight sensor data nodes and four repeaters-are used in the system, and they are connected to a gateway via a SmartMesh IP manager. The sun, dust, rain, and snow directly hit the wireless sensor network. There have been gathered data using the sensor equipment every ten seconds at four various heights (1, 2, 3, and 4 metres heights from the surface/ground). Ten meteorological stations' data on temperature and humidity are also utilised. These stations are close to the orchard, and the data is organised as a graph together with the orchard. Every hour, this data is gathered.

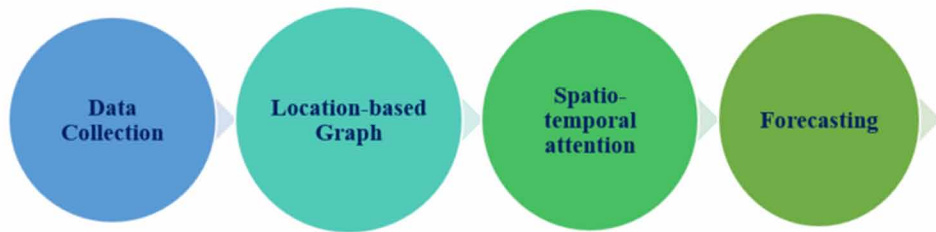
Using data from sensors and meteorological stations, we create the GSTA\_RGC model in this work to forecast the minimum temperature in the nearby experimental field for a set number of hours in the future. At a single time step, the graph for the stations is in Figure 16. This graph is expanded into a spatial-temporal graph over several time steps, where the feature values of each node are connected to their past, present, and geographical neighbours.



*Figure 16. Graph for the stations*



*Figure 17. Processes of GNN spatial-temporal graph model for frost forecast*



Now arranged the notation, where number  $n$  represents the nodes. The three dimensions of the training data are  $\{\text{temp, hum}\}$ , time  $t$ , and  $n$ . To predict the subsequent  $t$  steps, the model employs a window of  $T$  steps.

**Step 1:** Input data processing

**Step 2:** GNN that models geographical interactions

**Step 3:** Spatio-temporal attention that captures relevant spatial and temporal features

**Step 4:** Recurrent graph convolution to perform the forecasting.

Actional Forecasting techniques model comparison is shown in Table 2. For requiring frost forecasting over 6, 12, and 24 hours, the suggested model performs better than all examined baselines. It is clear that an autoencoder with an attention mechanism performs better than a GNN with spatiotemporal attention utilising convolution and GRU. For modelling geographical and temporal interactions, it is important to gather more weather data, extra weather variables, and employ more weather stations in order to enhance these findings.

Table 2. Time series forecasting models' average MAE and RMSE when used to forecast frost.

Model	MAE			RMSE		
	6hr	12hr	24hr	6hr	12hr	24hr
FNN	4.26	4.75	5.72	7.85	8.62	10.78
STA_C	3.75	4.05	4.85	6.50	8.05	8.70
STA_GRU	3.50	3.75	4.15	6.15	7.18	7.35
GSTA_RGC	3.05	3.24	3.87	5.44	5.80	6.15

Our frost forecasting model utilises a GNN architecture with a recurrent graph convolution technique to handle numerous time series simultaneously while optimising the graph structure between them. Spatiotemporal attention is added to the model to take spatial relationships into account and extract temporal dynamics.

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# Chapter 10

## Applications of GNNs and m-Health for Disease Tracking

**Ab Qayoom Sofi**

*Lovely Professional University, India*

**Ram Kumar**

*Lovely Professional University, India*

**Monica Sankat**

*Lovely Professional University, India*

### ABSTRACT

*The lifestyle of people across the globe has become fast and faulty, which has resulted in a highly stressful life full of anxiety and depression. People's habits have become very unhealthy, which has led to huge rise in several Non-Communicable diseases (NCDs) or lifestyle disorders like diabetes, hypertension, cardio vascular diseases, mental health issues, etc. The heart disease is still the biggest cause of mortality in the world. It is spreading at an alarming rate due to bad lifestyles, consumption of junk food, smoking, drinking, and lack of awareness and alertness. These lifestyle disorders are spreading at an alarming rate and are spreading from epidemic to a pandemic. These, besides other health consequences, have serious social and economic implications for the individual and for the country. These conditions have multiple dimensions and can be controlled and prevented if diagnosed and treated in time by improving the overall personality of an individual with the help of technology and self-management.*

### INTRODUCTION

The life style of people has changed drastically across the world and the people have adopted a very fast and stressful life with no balance between life and services. Their habits have become unhealthy which has caused several life style disorders like diabetes, hypertension, dyslipidemia, cardio vascular diseases and mental health issues. As per research statistics, an estimated 425 million people globally have diabetes accounting for 12% of the world's health expenditure and yet 1 in 2 persons remain undiagnosed

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and untreated. India has become the capital of diabetes and more than 30 million people are suffering from diabetes and many others are under the risk. One in every 10 individuals would be suffering from diabetics by the year 2040. Similarly, according to another statistics, nearly 17 million people die from cardiovascular disease every year, accounting for about 31% of the global deaths. The WHO has predicted that the Heart Disease will be the most silent killer of human being at least up to 2030. Diabetes or blood sugar or cardio vascular diseases, if left uncontrolled, can cause serious health problems ranging from severe damage and complications to the vital organs to the disability or even death.

Various deep learning techniques especially its recent architectures including GANs have the potential to deal with such problems in an efficient and reliable manner. Several latest deep learning techniques have already been deployed for the early and timely prediction of various chronic diseases. GNNs are one such type of deep learning techniques which can be effectively used to track and predict various kinds of chronic diseases on time. Further, these deep learning based working models can be converted into mobile apps or devices which can be integrated into mobiles or devices or smart watches etc. and can be made publicly accessible through Internet or IOT as almost everyone today possesses a mobile device and therefore everyone can be benefitted easily and everyone can take better care of his/her health. Already a number of such m-Health technologies have been approved by FDA. So, m-Health technologies can be used to implement GNNs in fast and effective manner. This study also aims to discuss how m-health technologies using GNNs can improve the prediction, diagnosis and effective self-management of chronic diseases especially in high risk patients and those suffering from infections and in worst conditions and pandemics like Covid-19.

Although there are several standalone apps, systems and devices developed for the self-management but all of these suffer from certain limitations as all of these work on only one or few aspects and factors. The goal of this study is to design and develop holistic devices for continuous real time monitoring of individuals for self-management to control chronic diseases like diabetes, cardio vascular diseases etc. This will not only help to identify and predict early if a normal person is at risk of developing a lifestyle disorder like diabetes, Cardio Vascular disease but will also help the patients to avoid any critical condition in the future by suggesting and recommending suitable actions in the form of reminders, notifications, SMS alerts etc.

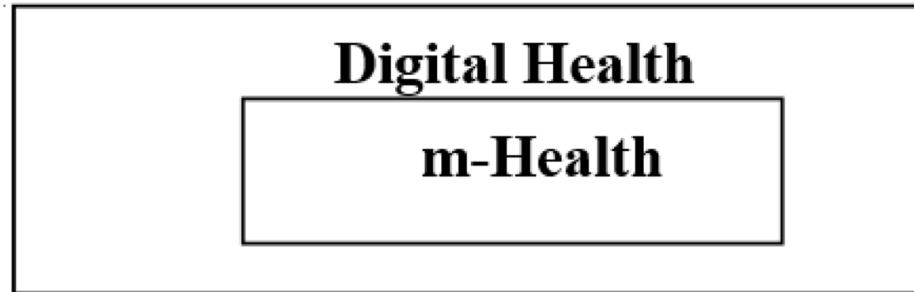
## **BACKGROUND**

According to US Food & Drug Administration (FDA), the delivery of health services and improvement in health outcomes via mobile and wireless devices is m-Health. m-Health interventions include AIDS, i.e., smartphone applications/apps, intelligent wearable technologies, devices and systems/services like Short Message Service (SMS). The subset of digital health or electronic health (e-Health) in which health information technology, telemedicine and personalized medicine are also included is m-health is as shown in Figure 1.

Digital Health Information Technology (HIT) is the future now owing to its adaptability to changed medical guidelines and translatability across different conditions. Further, e-Health is also quickly scalable to reach thousands of people and has tremendous potential to increased access to health care. Also, the major impact of Corona Virus pandemic of 2019 has made mobile and remote technologies indispensable for life. Life services have become dependent on technology which can provide better and

improved quality services to the users easily in real time, without human intervention. Deep learning techniques like GANs and GNNs are best suited and can be explored for such apps/agents, intelligent devices and systems/services (AIDS).

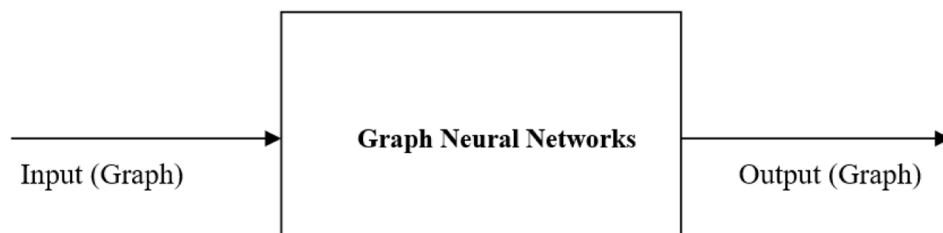
*Figure 1. m-health technologies*



## **DEEP LEARNING AND GRAPH NEURAL NETWORKS (GNNs)**

Almost everything in this universe can be represented in the form of Graphs, which can be processed by the deep learning neural networks called Graph Neural networks at much faster speeds. GNNs are actually the extension of simple deep learning neural networks whose input is a graph and output are also a graph as depicted in Figure 2.

*Figure 2. Graph neural networks*



It means almost all human problems can be solved by deep learning through Graph neural networks and that too with almost no human intervention. All we need to do is to convert an object or problem into a graph and feed it to a Graph Neural network for processing to produce the result, which again will be a graph and can be processed by other GNNs. So, pipelining and parallel processing of such problems/tasks can be done easily for obtaining the results quickly and efficiently. There are two common graph-based ML methods (for two levels) which are shallow embedding and graph neural networks (GNN).

With the advances in research, machine learning and more specifically deep learning algorithms have been potentially explored and applied to analyse health care data for the prediction of several diseases. One of the limitations of these methods is that most of these existing techniques use grid-like data, although, the data obtained from the physiological systems is generally irregular and unordered, which can be better represented through graphs. Hence, the graph-based models are ideally suitable and can be exploited to develop better models for the purpose and have, therefore, attracted great attention recently.

Disease prediction using graph machine learning is a promising approach that utilizes electronic health data to identify patterns and predict the onset of diseases in patients. This method involves constructing a graph-based representation of a patient's health records and applying machine learning algorithms to analyze the graph's structure and identify relevant features.

Graph-based models offer several advantages over traditional machine learning approaches, such as the ability to capture complex relationships between variables and the ability to incorporate heterogeneous data sources into a single model. This makes it an ideal approach for disease prediction, where a patient's health status is influenced by multiple factors, including genetics, lifestyle, and environmental factors.

The success of disease prediction using graph machine learning depends on the availability and quality of electronic health data. This includes clinical notes, lab results, imaging data, and genetic data, among others. These data sources are often soiled in different electronic health record systems, making it challenging to create a comprehensive patient profile. One of the key challenges in disease prediction using graph machine learning is the need for interpretable models that can be used to guide clinical decision-making. This requires developing methods for extracting meaningful insights from the graph-based models and presenting them in a way that is accessible to clinicians dynamically.

Despite these challenges, there have been several successful applications of disease prediction using graph machine learning, including predicting the onset of Alzheimer's disease, heart failure, and diabetes. As electronic health data becomes more widely available and machine learning algorithms become more sophisticated, we can expect to see further advances in this field, with the potential to revolutionize the way we approach disease prevention and treatment.

## **LITERATURE REVIEW**

According to a report, in 2018, smartphone is owned by approx. 66% of world's population including up to 80% in western European countries and 77% in USA. The clinicians can frequently contact with patients to provide the health information at the right time to facilitate self-management. So, m-Health technology is best suitable and can be easily applied to numerous areas including self-management of diabetes, Heart disease etc. Further, it has a potential for expanding and growing rapidly (El-Sappagh et al., 2019).

Managing life style disorders like diabetes, Heart disease is very challenging for both patients as well as clinicians. For self-managing successfully, patients must have high level of knowledge about the condition/status of the disease. Clinicians also need to frequently interpret glucose/Blood Pressure patterns/trends and adjust medication doses and recommend behavioral changes accordingly.

In 2014, there has been an increase in the occurrence of Type 2 diabetes (T2DM) dramatically across the globe to 8.5% of the population. It incurs huge human, economic and social costs besides inflicting significant burden on society in the shape of low productivity, increased healthcare expenses, premature mortality and intangible costs in the form of a poor quality of life. The expenditures on adults due to

diabetes were approximately \$727 billion, which account for about 12% of the global healthcare expenses in 2017 (Perveen et al., 2019).

According to the International Diabetes Federation (IDF), there were approximately 463 million people (20– 79 years) suffering from diabetes globally in 2019, and the number is expected to go further to 700 million by 2045. It is widely known that besides medications, lifestyle managements such as exercise, diet, and weight control, are necessary for treating disease. With recent advances in mobile technology, a large number of smartphone applications (apps) have been developed with the goal for facilitating self-management of diabetes mellitus (DM) (Park et al., 2020).

One of the biggest challenges with medical problems like diabetes, cardio vascular diseases is that it is very difficult to get access to the real-world data sets for developing high performance and accurate prediction models and tools for such disorders due to the privacy and confidentiality issues associated with these data sets. So, the experimental models tested on the standard data sets need to be used for developing web applications for the self-management of these diseases, which otherwise need to be highly specific and personalized as per the actual data in real time.

Using decision support systems may recommend data-driven actions that need final approval by the physician or patient but once implemented can improve patient outcome. So far, there has been only moderate reduction in HbA1c as per multiple studies and only borderline cost effectiveness through digital diabetes care, but the patient satisfaction and expectations are already on rise. The m-health technology and this study aims to integrate all digital patient data and provide personalized virtual or face-to-face visits to such persons as are in great need. However, different barriers to digital diabetes care/m-health technologies need to be understood in a better way and unmet needs to be identified in order to improve use of this growing and evolving technology in a safe and cost-effective manner (Kaufman et al., 2019).

## **RECOMMENDATIONS AND DISCUSSION**

Such diseases are actually chronic conditions and life style problems which involve a number of factors discussed and classified herein below. It is recommended that such m-health technologies or AIDS be designed and developed using deep learning and GNNs which could be applied in the real life for improving the life style of a person through self-management and tracking the disease and predicting it much earlier than it actually occurs.

### **Uncontrollable Factors**

Heredity is an uncontrollable risk factor which cannot be modified.

### **Controllable Factors**

However, there are a number of other risk factors which can be controlled by modifying the life style. These are listed below:

1. Stress
2. Sleep
3. Diet

4. Exercise
5. Weight
6. Emotions

The life style management for its improvement through m-health can be done as discussed below.

### **Stress Management**

It is most important for any person to live a happy and peaceful stress-free life in order to remain healthy and disease free. So, it is even more important for patients to remain stress and worry free as it has been studied that there is a strong correlation between stress levels and blood sugar levels. A happy and satisfied and grateful person is less likely to have the disease than the one who is not satisfied with life and always remains tense and under stress (Cahn et al., 2018).

### **Relaxing and Sleep Management**

It is extremely important to relax and have a very good sleep/rest especially during the night to always remain fresh minded in order to stay focused during the working hours in order to be productive and qualitative, which in turn enhances the mood and happiness (Alexander Fleming et al., 2020).

### **Diet Management**

Having a balanced diet is another crucial factor that determines the health of an individual. Patients must have good control over their diet and must take good, hygienic and healthy diet accordingly as per the advice of their doctors, nutritionists or care takers besides maintaining good timely and hygienic dietary habits, especially in the breakfast as it keeps a person active throughout the day (El-Sappagh et al., 2019).

### **Exercise and Weight Management**

Regular exercise plays a significant role in controlling disease and maintaining an active lifestyle. Patients must do exercise of their choice regularly to keep a check on their weight in order to maintain a healthy weight and BMI. Even walking especially in the morning for at least 25-30 minutes a day is considered to be one of the best exercises, which needs to be done regularly (Chaki et al., 2020).

### **Emotions and Speech Management**

Controlling emotions/feelings and balancing one's thoughts and speech is one of the less understood and less discussed factors. It is very important to maintain good mood and social relationships while dealing and interacting with people especially sensitive persons including disabled, diabetics, women and children in particular. Trusting self as well as others and always thinking positive about oneself as well as others helps is necessary to avoid mood swings which, in turn, prevents a person from irritation, stress or depression like problems, as it has been found that patients are more depressive and vice-versa (Dankwa-Mullan et al., 2019).



## **Blood Sugar Level Management**

All these factors influence the personality of the individual and affect the blood sugar level continuously in real time. To maintain healthy Blood Sugar Levels (BSL), it is vital for diabetic patients to keep their Blood Sugar Level under check and strict control which makes it necessary for them to monitor their BSL continuously in real time to adjust their life style and behavior accordingly. This has become even more necessary that such patients self-monitor and self-manage their BSL after the pandemic of Covid-19 and could, therefore be, treated anytime remotely by the doctors to avoid the direct contact and even during the lockdown periods also. Evidently, the diabetic patients should no longer be dependent on their dependents to take care of themselves. Regular communication, education and feedback to/by the doctors, nutritionists, psychotherapists/ physiotherapists and other care givers, is however, very important to monitor and control BSL (Sowah et al., 2020).

## **COMPONENTS OF THE AIDS**

So, to improve the life style, the self-management system for the disease must have a holistic approach and must be an integrated technological solution. There have been several standalone apps, systems/ devices developed for the diabetes/Heart disease management but all of these suffer from limitations as all of these work on one or few aspects/factors while ignoring the other important aspects/factors, although all of these aspects/factors need to be controlled and managed through one system simultaneously in order to be effective and improving in the real time. Several other medical devices are dependent devices which need to be connected to the user before taking the readings (Alfian et al., 2018).

Time has come to design, develop and use the integrated digital health care technologies and systems/ devices for the effective management of such chronic diseases, the proposed structure of which has been shown in Figure 3.

So, a complete intelligent system/device with following components and features need to be designed and developed with following features.

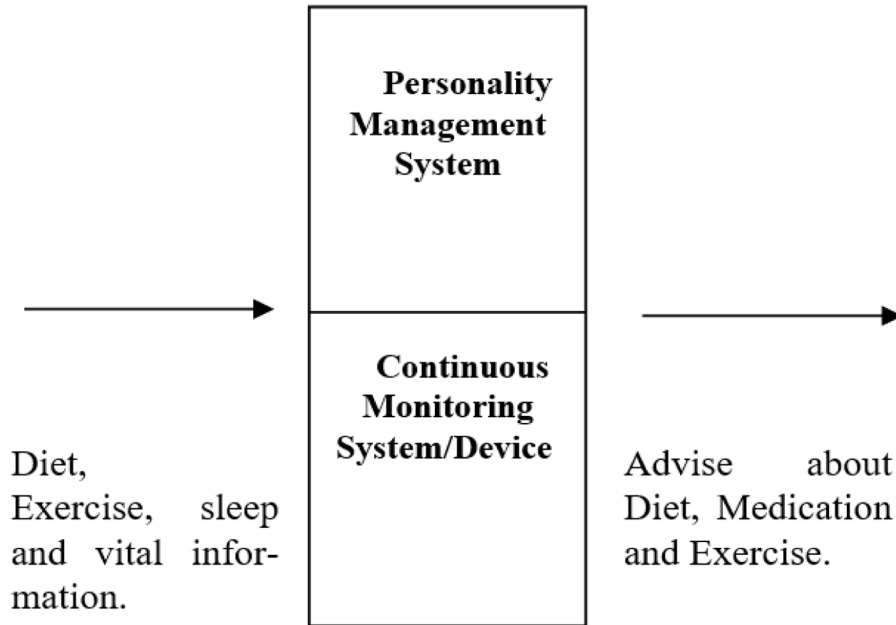
### **1. Social Support and Goal Setting:**

A person has to manage his overall personality to live and enjoy a happy stress-free life, which means people need to live a socially active life and have interaction and communication with family members, friends and society. It has been seen that people who don't have a social life tend to be more stressed, tense and less happy and have been found to have uncontrolled/less controlled blood sugar levels. So, diabetic patients need online social support in the form of voice calls, chatting, dating, gaming and surfing websites/portals or social networking sites. This module will also take care of the rest/sleep requirements of the user (Spänig et al., 2019).

### **2. Diet Management:**

This module is an AI based module that takes a picture of the meal before eating and determines whether it is healthy for the patient or not and advises/recommends the patient accordingly (Malasinghe et al., 2019).

*Figure 3. Structure of proposed integrated self-management system*



**3. Exercise Management:**

This component will provide information to the patient/user about how to control the weight and how much regular exercise is required to do so (Jung & Chung, 2016).

**4. Medication:**

This module will provide the advice about the change in the medicine or its dosage based on the blood sugar level (Benjamens et al., 2020).

**6. Education:**

The education module will provide general awareness to the users about the disease and about how to take better care of the self.

**7. Communication and Feedback:**

This is another important module that will ensure regular communication and feedback between the patient and care takers in the form of at least short messaging services (SMS) supported in all cell phones or in the form of voice and video calls supported by the smart phones.

## **BENEFITS AND FUTURE RESEARCH**

The quality of life of the patients could be greatly improved by the use of m-Health technologies and the diseases can be better controlled. Further, these can be used for the prevention of the disease by early detection of the disease from the patterns/trends. Below is the list of 29 AI/ML based medical technologies approved by FDA.

## **LIMITATIONS**

This study and system are dependent on mobile technology and therefore cannot be used by the people without access to mobile phones. Technology in the form of mobiles, social networking sites, dating sites and gaming platforms do provide an opportunity for people to connect and socialize online but excessive, unlimited and uncontrolled use of such apps/sites results in disadvantage rather than benefit and makes people addictive who therefore remain away from the natural and real life, which in turn may have negative impact. So, m-health technology must be used to manage the overall personality and not to control it (Ahmedt-Aristizabal et al., 2021). A well-managed and self-controlled or self-disciplined personality can make best use of m-health technology by balancing its timely use through proper time management. Although GNN-based models have achieved outstanding results as compared to the traditional ML methods in disease prediction tasks, they are still facing interpretability and dynamic graph challenges.

## **CONCLUSION**

It is necessary to keep the pandemic of diabetes/cardiovascular diseases and their financial consequences under control to lower the individual and national costs. There is a need to develop integrated digital systems/services/solutions/ m-IOT devices for the prevention, prediction and treatment of such diseases which are definitely better than the stand-alone applications. Deep learning has the immense potential to solve various complex problems faced by the mankind which humans could not have imagined earlier. Various deep learning techniques and its recent architectures like GANs and GNNS offer the solution by providing models that are easy to develop, fast and scalable which can be used for the early, accurate, reliable and efficient prediction of various diseases and can be easily converted into digital or mobile AIDS. So, m-Health technologies can improve the overall life style of the people and thereby improve the prevention and control of such chronic but fatal diseases. m-Health technologies are becoming more cost effective and scalable and are easy to implement because the underlying deep learning architectures are very fast, automatic and scalable. Though the disease prediction field using ML techniques is still emerging, GNN-based models have the potential to be an excellent approach for disease prediction, which can be used in medical diagnosis, treatment, and the prognosis of diseases.

*Table 1. Database of the FDA approved AI/ML-based medical technologies*

No.	Primary Medical Specialty/ Secondary Specialty	Month/Year	Name of Algorithm/Device	Algorithm Mentioned in the Announcement
1	Radiology/Cardiology	11/2016	Arterys Cardio DL	Deep Learning
2	Neurology	03/2017	EnsoSleep	Automated Algorithm
3	Radiology/Oncology	11/2017	Arterys Oncology DL	Deep Learning
4	Ophthalmology	01/2018	Idx	AI
5	Radiology/Neurology	02/2018	ContaCT	AI
6	Radiology/Emergency	02/2018	OsteoDetect	Deep Learning
7	Endocrinology	03/2018	Guardian Connect System	AI
8	Radiology/Cardiology	05/2018	EchoMD Automated Ejection Fraction	Machine Learning
9	Endocrinology	06/2018	DreaMed	AI
10	Radiology/Emergency Medicine	07/2018	BriefCase	Deep Learning
11	Radiology/Oncology	07/2018	ProFound™ AI Software V2.1	Deep Learning
12	Radiology	08/2018	SubtlePET	Deep neural network- based algorithm
13	Radiology/Oncology	09/2018	Arterys MICA	AI
14	Cardiology	09/2018	AI-ECG Platform	AI-ECG
15	Neurology	10/2018	Accipiolx	AI algorithm
16	Neurology	10/2018	icobrain	Machine Learning and Deep Learning
17	Internal Medicine	11/2018	FerriSmart Analysis System	AI
18	Radiology/Oncology	03/2019	cmTriage	AI
19	Radiology	04/2019	Deep Learning Image Reconstruction	Deep Learning
20	Radiology/Emergency Medicine	05/2019	HealthPNX	AI
21	Radiology	06/2019	Advanced Intelligent Clear-IQ Engine (AiCE)	Deep Convolutional neural network
22	Radiology	07/2019	SubtleMR	Convolutional neural network
23	Radiology	07/2019	AI-Rad Companion (Pulmonary)	Deep Learning
24	Radiology/Emergency Medicine	08/2019	Critical Care Suite	AI
25	Radiology	09/2019	AI-Rad Companion (Cardiovascular)	Deep Learning
26	Cardiology/Radiology	11/2019	EchoGo Core	Machine Learning based algorithm
27	Radiology/Oncology	12/2019	TrasnparaTM	Machine Learning Components
28	Radiology/Oncology	01/2020	QuantX	AI
29	Cardiology	01/2020	Eko Analysis Software	Artificial neural network

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# Chapter 11

## A Comprehensive Study on Student Academic Performance Predictions Using Graph Neural Network

**Kandula Neha**

*Lovely Professional University, India*

**Ram Kumar**

*Lovely Professional University, India*

**Monica Sankat**

*Lovely Professional University, India*

### ABSTRACT

*Predicting student performance becomes tougher thanks to the big volume of information in educational databases. Currently, in many regions, the shortage of existing system to investigate and monitor the coded progress and performance isn't being addressed. First, the study on existing prediction methods remains insufficient to spot the foremost suitable methods for predicting the performance of scholars in many institutions. Second is because of the shortage of investigations on the factors affecting student achievements particularly courses within specified context. Therefore, a systematic literature review on predicting student performance by using data processing techniques is proposed to enhance student achievements. The objective of this work is to supply an outline on the info techniques to predict student performance. Previous studies have extensively reported on optimizing performance predictions to highlight risky students and promote the achievement of good students. There are also contributions that overlap with various research fields.*

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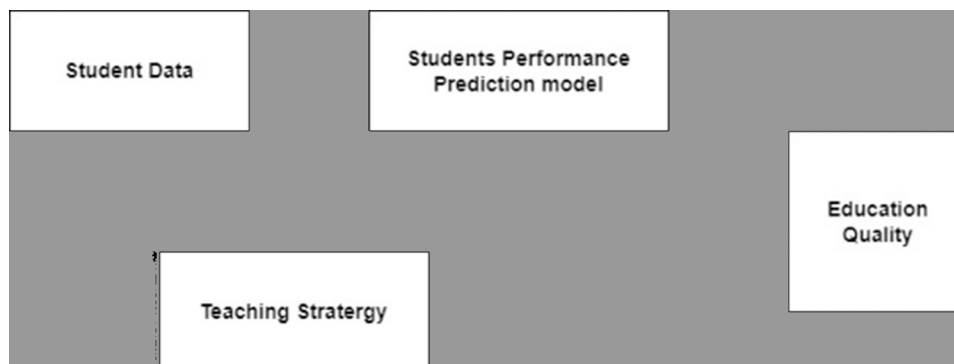
## INTRODUCTION

Student performance is the most important indicator of educational progress in any country. Student performance at school is greatly influenced by gender, age, teachers, and student learning. Predicting student performance is of great interest to education. In other words, student achievement refers to the degree to which a student achieves both immediate and long-term learning goals (Yadav & Pal, 2012). Good academic performance is an integral part of a quality university based on rankings. As a result, if the institution has strong achievements and academic performance, their ranking will improve. From a student's perspective, academic excellence is one of the most important aspects valued by employers, so maintaining academic excellence increases employment opportunities (Shahiri et al., 2015).

Predicting and analysing student performance is important to help educators identify their weaknesses and improve their performance. Similarly, students can improve their learning activities and managers can improve their processes (Mueen et al., 2016; Ashraf et al., 2018). By predicting student performance in a timely manner, educators can identify poor-performing individuals and intervene early in the learning process to apply the necessary interventions. Graph Neural Network is a new approach with a large number of applications that can make predictions about the data (Kushwaha et al., 2020). Educational data mining, ML techniques and Neural network techniques aim to model and recognize meaningful hidden patterns and available information from the educational context (Salah et al., 2020). In addition, academia applies the graph neural networks approach to large datasets, representing different student characteristics as data points. These strategies benefit different disciplines by achieving different goals such as pattern extraction, behaviour prediction, and trend discovery (Marbouti et al., 2015), providing educators with the most effective learning methods. Allows you to track and monitor student progress.

In the Internet of Everything environment, graphs have a powerful ability to do this. Represents functional relationships between students in the context of education graph. The structure naturally exists among students. Traditional performance prediction method Unable to handle this type of graph structure and ability to harness its potential. The relationships between students are very limited. This study Predict student performance based on the Graph Neural Networks (Figure 1). Our study was primarily motivated by the lack of a systematic and comprehensive study to assess student performance predictions using a variety of Graph Neural Network models. Therefore, the main purpose of this work was to collect and summarize the key predictive functions and networks used to predict student performance.

*Figure 1. Flow chart for basic student prediction model*





## LITERATURE REVIEW

### Predict Student Performance Based on Classical Machine Learning Methods

Predicting student learning outcomes is a difficult task for educational systems. Since so many researchers have used different Machine learning Classification techniques and Neural Networks in order to capture significant methods which are impacting in student academic performance:

Students' performance prediction may be a difficult task facing instructional systems.

The author provides a short summary of the present progressive performance prediction research. we have a tendency to 1st describe the present works on analysis mistreatment ancient machine learning strategies. (Marbouti et al., 2015) created 3 supplying regression models to spot at-risk students in a very giant first engineering course at 3 vital times of the semester in step with the educational calendar. The results show that the models were able to determine at-risk students early within the information. Martinho et al. proposed an intelligent system for student dropout prediction mistreatment the Fuzzy-ARTMAP neural network. the topics of the study area unit students from completely different technical faculties.

The research results show that the accuracy of the planned system is healthier than 76%, creating it potential to spot students UN agency might drop out early. (Riestra et al.,2021) used 5 machine learning algorithms (decision trees, naive Thomas Bayes, supplying regression, multilayer perceptron, and support vector machines) to make models to predict students' performance early by analysing huge LMS log info. They conjointly used a cluster algorithm to observe six completely different student teams and analyse the interaction mode of each cluster. To reveal the link between web usage behaviour and tutorial performance, Xu et al. (2019) verified the effectiveness of predicting tutorial performance from college students' web usage information employing a call tree, a neural network and a support vector machine. Arsad et al. (2013) studied the applying of a man-made neural network (ANN) model within the prediction of the educational performance of engineering students at Mara University of technology. Waheed et al. measured the effectiveness of clickstream data in a very virtual learning surroundings to predict insecure students through deep learning models and provided measures for early intervention. It's found that the prediction accuracy of deep artificial neural networks is healthier than baseline supplying regression and support vector machine models.

The high failure rate of scholars in introductory programming courses has aroused the vigilance of the many educators. Costa et al. used EDM technology to early determine students UN agency might fail introductory programming courses. They studied and evaluated the effectiveness of 4 prediction technologies (support vector machine, call trees, neural network and naive Bayes) on 2 completely different information sources in programming courses provided by Brazilian public universities. when applying data pre-processing and rule fine-tuning, the effectiveness of some technologies has been improved, and therefore the result of support vector machines achieved the simplest results.

Other analysis works propose new prediction strategies supported machine learning techniques to boost the accuracy of performance prediction. Ren et al. developed a personalized linear multiple correlation (PLMR) model to predict student performance. The model tracks student engagement in MOOCs in period of time through clickstream server logs and predicts student performance within the course. Yang et al. used the coed attribute matrix (SAM) to create a student model with score-related attributes and nonscore-related attributes to quantify student attributes for more analysis. They planned a student performance estimation tool supported classification BP-NN (back propagation neural network) which

may estimate student performance in step with students' previous knowledge and different student performance indicators with similar characteristics.

Chui et al. (2020) planned a reduced coaching vector-based support vector machine (RTVSVM) to predict at-risk and marginal students.

The model will cut back the coaching vector and shorten the coaching time while not touching classification accuracy. To convert students' course participation into pictures for early warning and prediction analysis, Yang et al. proposed 2 innovative methods: monaural learning image recognition (1-CLIR) and three-channel learning image recognition(3-CLIR). A learning image refers to a graph of all the information collected within the learning method, as well as behavior, text and different recordable data. The results show that each strategy will considerably capture additional insecure students than support vector machines, random forest and deep neural networks. Table 1 lists some common techniques and strategies for predicting performance.

Table 1 is list of some techniques used for prediction purpose.

*Table 1. Techniques used for prediction purpose*

<b>Problem Formulation</b>	<b>Techniques/Models</b>
Students' early performance prediction (Arsad et al., 2013)	Artificial Neural Network (ANN)
Predicting dropout students (Costa et al.,2017)	Fuzzy-ARTMAP Neural Network
Identify at-risk students (Marbouti et al., 2015)	Logistic Regression (LR)
Predicting student performance in MOOCs (Ren et al., 2016)	Personalized linear multiple regression model
Early prediction of students' academic failure in introductory programming courses (Fonseca et al., 2017)	Support Vector Machine (SVM)
	Decision Tree
	Neural Network
	Naive Bayes
Predicting at-risk and marginal students (Chui et al., 2020)	Reduced training vector-based SVM
Predicting academic performance from college students' Internet usage data (Xu et al.,2019)	Decision Tree
	Neural Network
	Support Vector Machine
Recognize learning images for early warning of at-risk students (Yang et al., 2020)	Convolutional Neural Network (CNN)
Early prediction of course-agnostic student performance (Riestra et al., 2021)	Decision Trees
	Naive Bayes
	Logistic Regression (LR)
	Multilayer Perceptron (MLP)
	Support Vector Machine (SVM)

## GRAPH NEURAL NETWORK APPLICATIONS IN EDUCATION

In recent years, neural networks (GNNs) or more generally deep learning have been graphed. Graphene has received a lot of attention because of its amazing potential. When analysing non-lattice structure

data that can be represented as a graph (Nakagawa et al., 2019, Song et al., 2021). As a powerful tool for processing chart data, GNN has been used in a variety of applications such as social networks, recommender systems, computer vision, and nature. Language processing, chemistry, biology, etc. (Yang et al., 2020; Abdelrahman et al., 2021; Gan et al., 2022).

With the event of intelligent education (i.e., “AI + Education” during a broad sense), GNNs and associated deep learning techniques for graphs are utilized underneath various situations within the education domain. as an example, data following (KT) aims to track students’ organic process mastery of specific data or ideas in step with their historical learning interaction with corresponding exercises. (Nakagawa et al., 2019) applied GNNs to data following for the primary time and planned a GNN-based data tracing technique (GKT) that transforms the data structure into a graph to rework the data following task into a time-series node-level classification drawback in GNNs. Since data graph structures aren’t expressly provided in most cases, the authors also propose numerous implementations of graph structures.

Song et al. (2021) planned a joint graph convolutional network-based deep data tracing (JKT) technique that adopts a unique inference-generating data tracing framework. JKT sculptures the multidimensional relationship between “exercise-to-exercise” and “concept to concept” into a graph and coalesced them with “exercise-to-concept” relationships to deal with the problems such as the problem models expertise capturing the semi-permanent dependency of student exercise history and modelling the interactions between student-questions and student skills during a consistent method. Yang et al. (2020) planned a graph-based interaction model for knowledge tracing (GIKT) that utilizes GCN to considerably incorporate question-skill correlations via embedding propagation. Taking into consideration the students’ forgetting behavior, (Abdelrahman et al., 2021) conferred a unique data tracing model, named deep graph memory network (DGMN) which includes a forget gating mechanism into the attention memory structure to dynamically capture forgetting behaviour throughout data tracking.

Cognitive identification is another basic issue in intelligent academic settings which aims to diagnose students’ data proficiency. (Gao et al., 2018) planned a novel relation map-driven psychological feature identification (RCD) framework that unifies modelling interactive and structural relations through a multi-layer student-exercise-concept map. (Mao et al.,) planned a learning behavior-aware psychological feature identification (LCD) framework for students’ psychological feature modelling with each learning behavior records and exercise records, where GCN is employed to mechanically refine the feature vectors representing exercises and videos. (Zhang et al., 2019) planned a graph-based data tracing increased psychological feature diagnosis model (GKT-CD) and improved the performance of psychological feature medicine for both the coed issue and exercise issue. GKT-CD carries out psychological feature identification underneath a cooperative framework that is developed to trace the student-knowledge response records and extract students’ latent traits.

Automatic short answer grading (ASAG) could be a challenging task geared toward predicting the score of a given student’s response. (Tan et al., 2021) used a two-layer GCN to encrypt the directionless heterogeneous graphs of all students’ answers. In terms of performance prediction, researchers utilised the applying potential of GNNs. Hu et al. (2020) planned a brand new GCN model supported attention to capture the advanced graph structure data evolution conferred by student knowledge to predict students’ performance in future courses.

Karim et al. (2020) developed a model named deep on-line performance analysis (DOPE) to predict students’ course performance in online learning. DOPE 1st models the coed course relations within the on-line system as a data graph then extracted the course and student embedding victimization the GNNs, encoded the temporal student behavioural knowledge of scholars within the system victimization the

recursive neural network, and eventually foretold the performance of scholars during a given course. Li et al. (2020) established the link model between students and issues using student interaction, they made the coed interaction drawback network, and further planned a brand new GNN model, referred to as R2GCN.

The model is actually applicable to heterogeneous networks and might understand generalized student performance prediction in interactive on-line question pools. Table 2 is a pair of lists typical applications of GNN in education.

*Table 2. Techniques and model management*

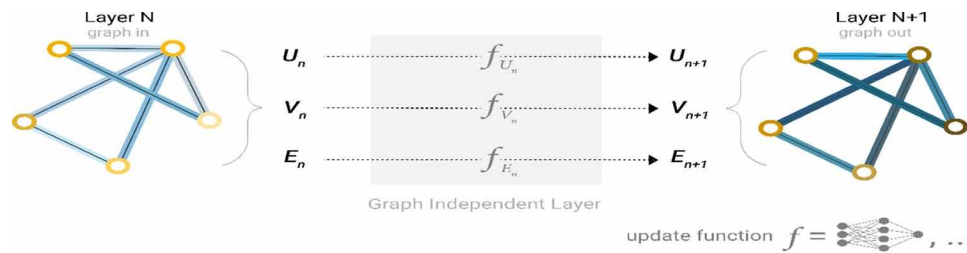
Techniques and Model Used	Application
Graph-based knowledge tracking model (GKT), 2019	Knowledge Tracking
Graph-based interaction model for knowledge tracing (GIKT),2020	
Joint graph convolutional network based deep knowledge tracing (JKT) 2021	
Attentive knowledge tracing based on graph representation learning (KS-GKT) 2021	
Deep graph memory network (DGMN) 2021	
Bi-Graph contrastive learning-based knowledge tracing (Bi-CLKT) 2022	
Relation map driven cognitive diagnosis (RCD) 2021	Cognitive Skills
Learning behavior perception cognitive diagnosis (LCD) 2021	
Cognitive diagnosis model enhanced by graph-based knowledge tracing (GKT-CD) 2021	
Graph convolutional network 2020	Automatic Short answer grading
Attention-based graph convolutional networks 2019	Performance Prediction
Relational graph convolutional neural network 2020	
Residual relational graph neural network 2020	

## GRAPH NEURAL NETWORKS

A GNN is Associate in nursing optimizable transformation on all attributes of the graph (nodes, edges, global-context) that preserves graph symmetries (permutation invariances). We're progressing to build GNNs victimization the "message passing neural network" framework projected victimization the Graph Nets design schematics introduced by Battaglia et al. GNNs adopt a "graph-in, graph-out" design which means that these model varieties settle for a graph as input, with data loaded into its nodes, edges and global-context, and more and more remodel these embedding's, while not ever-changing the property of the input graph (Figure 2).

With the numerical illustration of graphs that we've made higher than (with vectors rather than scalars), we have a tendency to square measure currently able to build a GNN. we are going to begin with the best GNN design, one wherever we have a tendency to learn new embeddings for all graph attributes (nodes, edges, global), however wherever we have a tendency to don't nonetheless use the property of the graph.

Figure 2. Basic GNN model

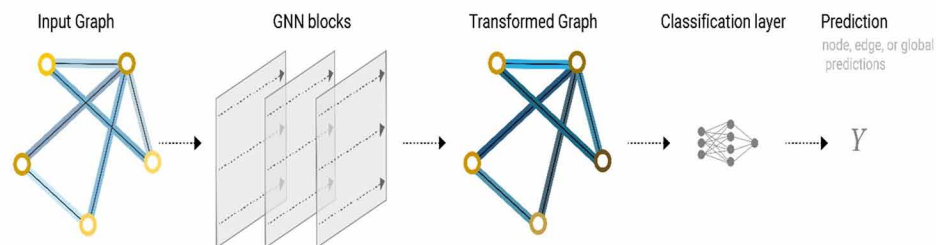


For simplicity, the previous diagrams used scalars to represent graph attributes; in apply feature vectors, or embeddings, square measure way more helpful. This GNN uses a separate multilayer perceptron (MLP) (or your favourite differentiable model) on every part of a graph; we have a tendency to decision this a GNN layer. for every node vector, we have a tendency to apply the MLP and obtain back a learned node-vector. we have a tendency to do a similar for every edge, learning a per-edge embedding, and conjointly for the global-context vector, learning one embedding for the whole graph.

As is common with neural networks modules or layers, we will stack these GNN layers along. Because a GNN doesn't update the property of the input graph, we will describe the output graph of a GNN with a similar nearness list and therefore the same range of feature vectors because the input graph. But, the output graph has updated embedding's, since the GNN has updated every of the node, edge and global-context representations.

## GNN Prediction by Pooling Information

Figure 3. GNN pooling



We will contemplate the case of binary classification; however, this framework will simply be extended to the multi-class or regression case. If the task is to form binary predictions on nodes, and also the graph already contains node info, the approach is straightforward—for every node embedding, apply a linear classifier (Figure 3).

However, it's not forever thus straightforward. As an example, you may have info within the graph hold on in edges, however no info in nodes, however still have to be compelled to build predictions on nodes. We want how to gather info from edges and provides them to nodes for prediction. We are able to do that by pooling. Pooling issue in 2 steps:

For each item to be pooled, gather every of their embedding's and concatenate them into a matrix.

The gathered embedding's square measure then collective, sometimes via a total operation. For a lot of in-depth discussion on aggregation operations move to the examination aggregation operations section. We represent the pooling operation by the letter  $\rho$ , and denote that we tend to square measure gathering info from edges to nodes as

$$\rho E_n \rightarrow V_n.$$

## Passing Message Between Graphs

We might build a lot of refined predictions by exploitation pooling at intervals the GNN layer, so as to create our learned embeddings tuned in to graph property. we are able to try this exploitation message passing, wherever neighbouring nodes or edges exchange data and influence every other's updated embeddings.

Message passing works in 3 steps:

- For each node within the graph, gather all the neighbouring node embedding's (or messages), that is that the perform delineate higher than.
- Aggregate all messages via associate mixture perform (like sum).
- All pooled messages are passed through more experienced responsible established an update perform, sometimes a learned neural network.

You could additionally 1) gather messages, 3) update them and 2) mixture them and still have a permutation invariant operation. Just as pooling may be applied to either nodes or edges, message passing will occur between either nodes or edges. These steps are key for leverage the property of graphs. We'll build a lot of elaborate variants of message passing in GNN layers that yield GNN models of accelerating quality and power.

## Graph Convolutions as Matrix Multiplications and Matrix Multiplications as Walks on a Graph

The first purpose we wish associate degree example as associate instance let's say is that the matrix operation of an adjacent matrix  $A$   $n_{\text{nodes}} \times n_{\text{nodes}}$  with a node feature matrix  $X$  of size  $n_{\text{nodes}} \times n_{\text{dim}}$  implements an straightforward message passing with a summation aggregation.

Let the matrix be  $B = AX$ , we will observe that any entry  $B_{ij}$  may be expressed as

$$= A_{i,1}X_{1,j} + A_{i,2}X_{2,j} + \dots + A_{i,n}X_{n,j} = \sum_k A_{i,k} X_{k,j}.$$

Because  $A_{i,k}$  area unit binary entries only if a edge exists between node  $i$  and node  $k$ , the real number is basically "gathering" all node options values of dimension  $j$  that share a position with node  $i$ . It ought to be noted that this message passing isn't change the illustration of the node options, simply pooling neighbouring node options. However, this will be simply custom-made by-passing  $X$  through your favourite differentiable transformation (e.g. MLP) before or when the matrix multiply.

From this, we will appreciate the advantage of exploitation contiguousness lists. Because of the expected sparseness of  $A$  we have a tendency to don't have to be compelled to total all values wherever  $A_{i,j}$  is zero. As long as we've got associate operation to assemble values supported associate index, we must always be ready to simply retrieve positive entries. to boot, this matrix multiply-free approach frees USA from exploitation summation as associate aggregation operation.

We can imagine that applying this operation multiple times permits USA to propagate data at larger distances. during this sense, matrix operation may be a kind of traversing over a graph. This relationship is additionally apparent after we check up on powers Alaska of the contiguousness matrix. If we have a tendency to think about the matrix  $A^2$ , the term  $A^2_{ij}$  counts all walks of length two from node  $i$  to node  $j$  and may be expressed because the real number:

$$= A_{i,1}A_{1,j} + A_{i,2}A_{2,j} + \dots + A_{i,n}A_{n,j}.$$

The intuition is that the primary term  $a_i$  is barely positive below 2 conditions, there's edge that connects node  $i$  to node  $1$  and another edge that connects node  $1$  to node  $j$ . In alternative words, each edges kind a path of length two that goes from node  $i$  to node  $j$  passing by node  $1$ . Because of the summation, we have a tendency to area unit count over all doable intermediate nodes. This intuition carries over after we think about  $A^3 = AA^2$ .. so on to Alaska.

## DEEP LEARNING OF GRAPHS

The implementation of conception of Node Embedding. It means that mapping nodes to a  $d$ - dimensional embedding area (low dimensional area instead of the particular dimension of the graph), in order that similar nodes within the graph square measure embedded getting ready to one another.

Our goal is to map nodes in order that similarity within the embedding area approximates similarity within the network.

Neural Networks square measure given in gray boxes. They need aggregations to be order-invariant, like sum, average, maximum, as a result of their permutation-invariant functions (Figure 4). This property allows the aggregations to be performed.

Let's loco mote to the forward propagation rule GNNs. It determines however the data from the input can move to the output facet of the neural network.

So as to perform forward propagation during this process graph, we'd like three steps:

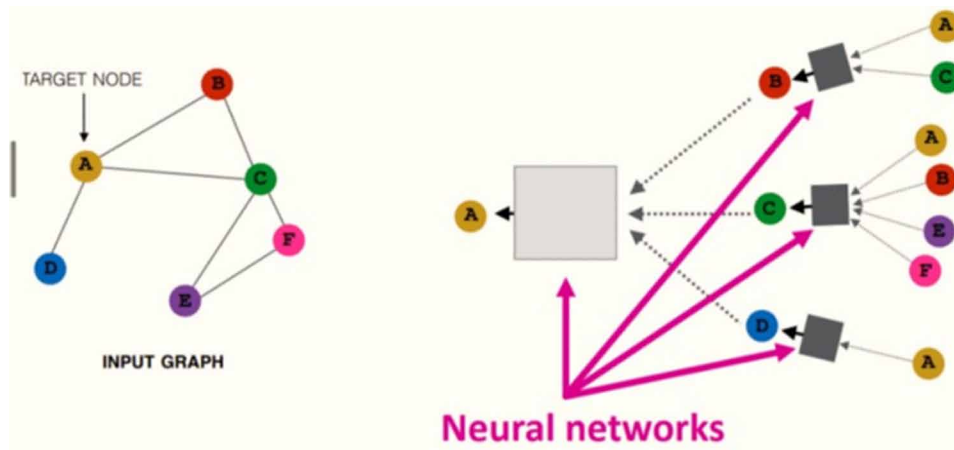
1. Initialize the activation units

$$h = x(\text{feature vector})$$

2. Each layer within the network

We can notice that three square measure 2 components for this equation.

Figure 4. Basic neural network with GNN



The first half is largely averaging all the neighbours of node  $v$ . The Second half is that the previous layer embedding of node  $v$  increases with a bias that may be a trainable weight matrix and it's essentially a self-loop activation for node  $v$ .

Training are often unattended or supervised

Unsupervised Training – Use solely the graph structure: similar nodes have similar embedding. Unattended loss perform are often a loss supported node proximity within the graph or random walks.

Supervised Training - Train model for a supervised task like node classification, traditional or abnormal node. To recap, during this we have a tendency to delineate a basic plan of generating node embedding by aggregating neighbourhood info.

## Graph Convolution Networks

GCNs were 1st introduced in “Spectral Networks and Deep domestically Connected Networks on Graphs” (Bruna et al., 2014), as a technique for applying neural networks to graph-structured information

The Simplest GCN has solely 3 totally different operators: Graph Convolution, Linear layer and Non-Linear Activation. The operators square measure sometimes worn out this order. Together, they create up one network layer. We will mix one or a lot of layers to make an entire GCN.

## APPLICATIONS OF GNN

Graph-structured information is implemented everywhere. The issues that GNNs resolve is classified into these categories:

**Node Classification:** The task here is to work out the labelling of samples (represented as nodes) by staring at the labels of their neighbours. Usually, issues of this sort area unit trained in a very semi-supervised method, with solely a vicinity of the graph being labelled.



**Graph Classification:** The task here is to classify the full graph into completely different classes. It's like image classification, however the target changes into the graph domain.

The applications of graph classification area unit varied associate degree vary from decisive whether or not a macromolecule is an accelerator or not in bioinformatics, to categorizing documents in IP, or social network analysis (Gilmer et al., 2017; Hamrick et al., 2018).

**Graph Visualization:** It is a district of arithmetic and technology, at the intersection of geometric graph theory and knowledge visual image. it's involved with the visual illustration of graphs that reveals structures and anomalies that will be gift within the information and helps the user to know the graphs.

**Link Prediction:** Here, the rule should perceive the link between entities in graphs, and it conjointly tries to predict whether or not there's a association between two entities. It's essential in social networks to infer social interactions or to recommend attainable friends to the users. it's conjointly been utilized in recommender system issues and in predicting criminal associations.

**Graph Bunch:** Refers to the clustering of knowledge within the variety of graphs. There are a unit of two distinct sorts of bunch performed on graph information. Vertex bunch seeks to cluster the nodes of the graph into teams of densely connected regions supported either edge weights or edge distances. The second variety of graph bunch treats the graphs because the objects to be clustered and clusters these objects supported similarity.

## **GNNs in Laptop Vision**

Using regular CNNs, machines will distinguish and determine objects in pictures and videos. Though there's still a lot of development required for machines to possess the visual intuition of a person's. Yet, GNN architectures is applied to image classification issues. One of these issues is scene graph generation, within which the model aims to analyse a picture into a linguistics graph that consists of objects and their linguistics relationships. Given a picture, scene graph generation models find and acknowledge objects and predict linguistics relationships between pairs of objects. However, the quantity of applications of GNNs in laptop vision continues to be growing. It includes human-object interaction, few-shot image classification.

## **GNNs in Linguistic Communication Process**

In NLP, we all know that the text could be a kind of serial information which may be delineate by associate degree RNN or associate degree LSTM. However, graphs area unit heavily utilized in varied IP tasks, because of their naturalness and easy illustration.

Recently, there has been a surge of interest in applying GNNs for an outsized range of IP issues like text classification, exploiting linguistics in AI, user geolocation, relation extraction, or question respondent. We know that each node is associate degree entity and edges describe relations between them. In IP analysis, the matter of question respondent isn't recent. However, it absolutely was restricted by the present information. Although, with techniques like Graphs age (Ruiz et al., 2020), the strategies is generalized to antecedent unseen nodes.

## **GNNs in Traffic**

Forecasting traffic speed, volume, or the density of roads in traffic networks is basically necessary in a very good transit. we will address the traffic prediction drawback by mistreatment STGNNs. Considering the traffic network as a spatial-temporal graph wherever the nodes area unit sensors put in on roads, the sides area unit measured by the space between pairs of nodes, and every node has the typical traffic speed among a window as dynamic input option.

## **GNNs in Chemistry**

Chemists will use GNNs to analysis the graph structure of molecules or compounds. In these graphs, nodes area unit atoms, and edges – chemical bonds.

## **GNNs in Alternative Domains**

The application of GNNs isn't restricted to the on top of domains and tasks. There are tries to use GNNs to a spread of issues like program verification, program reasoning, social influence prediction, recommender systems, electrical health records modelling, brain networks, and adversarial attack hindrance. Table 3 shows the different applications of GNN.

## **Generative Models of GNN**

Generative models for real-world graphs have drawn important attention for his or her necessary applications as well as modelling social interactions, discovering new chemical structures, and constructing information graphs. As deep learning strategies have powerful ability to be told the implicit distribution of graphs, there's a surge in neural graph generative models recently.

NetGAN (Shchur et al., 2018) is one among the primary work to create neural graph generative model, that generates graphs via random walks. It transforms the matter of graph generation to the matter of walk generation that takes the random walks from a selected graph as input and trains a walk generative model victimisation GAN design. whereas the generated graph preserves necessary topological properties of the initial graph, the quantity of nodes is unable to alter within the generating method, that is as same because the original graph (Zou et al., 2019). GraphRNN (You et al., 2018) manages to get the closeness matrix of a graph by generating the closeness vector of every node step by step (Hu et al, 2020), which may output networks with totally different numbers of nodes. Li et al. (2018) propose a model that generates edges and nodes consecutive and utilizes a graph neural network to extract the hidden state of this graph that is employed to come to a decision the action within the next step throughout the successive generative method. GraphAF (Shi et al., 2020) conjointly formulates graph generation as a successive call method (Han et al., 2018). It combines the flow-based generation with the autogressive model. Towards molecule generation, it conjointly conducts validity check of the generated molecules victimisation existing chemical rules once every step of generation (Wu et al., 2019).

*Table 3. Applications of GNN*

Application	Deep Learning	Description
Neural Machine Translation	Graph convolutional network/ gated graph neural network	The neural MT (NMT) is taken into account a sequence-to-sequence task. One in every of GNN's common applications is to include linguistics info into the NMT task. To do this, we tend to utilize the grammar GCN on syntax-aware NMT tasks. We are able to additionally use the GGNN in NMT. It converts the grammar dependency graph into a replacement structure by turning the perimeters into extra nodes and therefore edges labels is portrayed as embedding
Relation extraction	Graph LSTM/ graph convolutional network	Relation Extraction is that the task of extracting linguistics relations from the text, that sometimes occur between 2 or additional entities. ancient systems treat this task as a pipeline of 2 separated tasks, i.e., named entity recognition (NER) and relation extraction, however new studies show that end-to-end modelling of entity and relation is vital for top performance since relations move closely with entity info
Image classification	Graph convolutional network/ gated graph neural network	Image classification could be a basic pc vision task. Most of the models offer engaging results once given an enormous coaching set of labelled categories. The main focus now's towards obtaining these models to perform well on zero-shot and few-shot learning tasks. For that, GNN seems quite appealing. data graphs will offer the required info to guide the ZSL (Zero-shot learning) task
Object detection Interaction detection Region classification Semantic segmentation	Graph attention network Graph neural network Graph CNN Graph LSTM/ gated graph neural network/ graph CNN/ graph neural network	There are alternative applications of pc vision tasks like object detection, interaction detection, and region classification. In object detection, GNNs are accustomed calculate RoI features; in interaction detection, GNN is message-passing tools between humans and objects; in region classification, GNNs perform reasoning on graphs that connect regions and categories
Physics	Graph neural network/ graph networks	Modelling real-world physical systems is one in every of the foremost basic aspects of understanding human intelligence. By representing objects as nodes and relations as edges, we are able to perform GNN-based reasoning regarding objects, relations, and physics in a good method. Interaction networks is trained to reason regarding the interactions of objects in a very advanced physical system. It will create predictions and inferences regarding numerous system properties in domains like collision dynamics
Molecular fingerprints	Graph convolutional network	Molecular fingerprints are feature vectors that represent molecules. cc models predict the properties of a replacement molecule by learning from example molecules that use fixed-length fingerprints as inputs. GNNs will replace the standard implies that provides a fastened cryptography of the molecule to permit the generation of differentiable fingerprints custom-made to the task that they're needed
Protein interface prediction	Graph convolutional network	This is a difficult drawback with vital applications in drug discovery. The planned GCN-based technique severally learns matter and receptor macromolecule residue illustration and merges them for pairwise classification. At a molecular level, the perimeters is the bonds between atoms in a very molecule or interactions between amino-acid residues in a very macromolecule. On an oversized scale, graphs will represent interactions between additional advanced structures like proteins, mRNA, or metabolites
Combinatorial optimization	Graph convolutional network/ graph neural network/ graph attention network	Combinatorial improvement (CO) could be a topic that consists of finding Associate in Nursing optimum object from a finite set of objects. It's the bottom of the many vital applications in finance, logistics, energy, science, and hardware style. Most CO issues are developed with graphs. in a very recent work by DeepMind and Google, graph nets are used for 2 key subtasks concerned within the MILP solver: joint variable assignment and bounding the target worth. Their neural network approach is quicker than existing solvers on huge datasets
Graph generation	Graph convolutional network/ graph neural network/ LSTM /RNN/ relational-GCN	Generative models for real-world graphs have drawn important attention for his or her vital applications together with modelling social interactions, discovering new chemical structures, and constructing data graphs. The GNN primarily based model learns node embedding999 for every graph severally and matches them victimisation attention mechanisms. This technique offers sensible performance compared to straightforward relaxation-based techniques

Instead of generating graph consecutive, alternative works generate the closeness matrix of graph promptly. MolGAN (DeCao & Kipf, 2018) utilizes a permutation-invariant differentiator to unravel the node variant downside within the closeness matrix (Zhang et al., 2019). Besides, it applies a gift network for RL-based improvement towards desired chemical properties. What's additional, (Ma et al.2018) propose affected variational auto-encoders to make sure the linguistics validity of generated graphs. And GCPN (You et al., 2018) incorporates domain-specific rules through reinforcement learning. GNF (Liu et al., 2019) adapts normalizing flow to the graph information. Normalizing flow could be a reasonably generative model that uses an invertible mapping to rework discovered information into latent vector house. remodelling from the latent vector back to the discovered information victimisation the inverse matrix is the generating method. GNF combines normalizing flow with a permutation-invariant graph auto-encoder to require graph structured information because the input and generate new graphs at the check time. atomic number 6 (Grover et al., 2019) integrates GNN into variational auto-encoders to cypher the graph structure and options into latent variables. additionally specifically, it uses isotropic Gaussian because the latent variables then uses unvaried refinement strategy to decrypt from the latent variables (Cui et al., 2020) an existing GNN model to illustrated the planning method. Taking the task of heterogeneous graph pretraining as associate degree example, we tend to use GPT-GNN (Hu et al., 2020b) because the model parenthetically the planning method (Maehara, 2019).

1. **Find Graph Structure.** The paper focuses on applications on the tutorial information graph and also the recommendation system. within the educational information graph, the graph structure is express. In recommendation systems, users, things and reviews are often thought to be nodes and also the interactions among them are often thought to be edges, that the graph structure is additionally simple to construct.
2. **Specify Graph Kind and Scale.** The tasks specialize in heterogeneous graphs, so sorts of nodes and edges ought to be thought of and incorporated within the final model. because the educational graph and also the recommendation graph contain uncountable nodes, so the model ought to additional contemplate the potency downside. Finally, the model ought to specialize in large-scale heterogeneous graphs.
3. **Design Loss Operate.** As downstream tasks in Hu et al. (2020) square measure all node-level tasks (e.g., Paper-Field prediction within the educational graph), so the model ought to learn node representations within the pretraining step. within the pretraining step, no labelled information is accessible, so a self-supervised graph generation task is meant to be told node embeddings. within the fine-tuning step, the model is fine-tuned supported the coaching information of every task, so the supervised loss of every task is applied (Xu et al., 2019; Chen et al., 2020).
4. **Build Model Victimisation Process Modules.** Finally, the model is constructed with process modules. For the propagation module, the authors use a convolution operator HGT (Hu et al., 2020) that we tend to mentioned before. HGT incorporates the kinds of nodes and edges into the propagation step of the model and also the skip association is additionally side within the design. For the sampling module, a specially designed sampling technique Sampling (Hu et al., 2020) is applied, that could be a heterogeneous version of girls (Zou et al., 2019). because the model focuses on learning node representations, the pooling module isn't required. The HGT layer square measure stacked multiple layers to be told higher node embeddings.

## **Analyses of GNNs**

### **Graph Signal Method**

From the spectral perspective of browse, GCNs perform convolution operation on the input choices inside the spectral domain that follows graph signal method in theory.

There exist several works analysing GNNs from graph signal method. Li et al. (2018) initially address the graph convolution in graph neural networks is actually Laplacian smoothing, that smooths the feature matrix so as that close to nodes have similar hidden representations. Laplacian smoothing reflects the homophile assumption that close to nodes are imagined to be similar. The Laplacian matrix may be a low-pass filter for the input choices. SGC (Wu et al., 2019) a lot of removes the burden matrices and nonlinearities between layers, showing that the low-pass filter is that the explanation why GNNs work (Scarselli et al., 2018).

Following the conception of low-pass filtering, Zhang et al. (2019), Cui et al. (2020), Nt and Maehara (2019), and Chen et al. (2020) analyse wholly totally different filters and provide new insights. to appreciate low-pass filtering for all the eigenvalues, AGC (Zhang et al., 2019) designs a graph filter  $I - 12L$  in step with the frequency response operate. AGE (Cui et al., 2020) a lot of demonstrates that filter with  $I - 1\lambda_{\max}L$  might retrieve results, where is that the foremost eigenvalue of the Laplacian matrix (Garg et al., 2020) Despite linear filters, Graph Heat (Xu et al., 2019) leverages heat kernels for higher low-pass properties. NT and Maehara (Nt & Maehara, 2019) state that graph convolution is primarily a denoising methodology for input choices, the model performances heavily rely on the amount of noises inside the feature matrix. To alleviate the over-smoothing issue, Chen et al. (2020) gift a pair of metrics for live the smoothness of node representations and conjointly the over-smoothness of GNN models. The authors conclude that the information-to-noise relation is that the key issue for over-smoothing.

### **Generalization**

The generalization ability of GNNs have in addition received attentions recently. Scarselli et al. (2018) prove the VC-dimensions for a restricted class of GNNs. Garg et al. (2020) provide plentiful tighter generalization bounds supported Rademacher bounds for neural networks.

Verma and Zhang (2019) analyze the soundness and generalization properties of single-layer GNNs with wholly totally different convolutional filters. The authors conclude that the soundness of GNNs depends on the foremost vital eigenvalue of the filters. Knyazev et al. (2019) specialise in the generalization ability of attention mechanism in GNNs. Their conclusion shows that focus helps GNNs generalize to larger and yelling graphs (Knyazev et al., 2019).

### **Expressivity**

On the expressivity of GNNs, Xu et al. (2019) and Morris et al. (2019) show that GCNs and Graph SAGE are less discriminative than Weisfeiler-Leman (WL) check, Associate in Nursing rule for graph similarity testing. Xu et al. (2019) in addition propose GINs for added communicative GNNs. occurring the way aspect WL check, Barceló et al. (2019) discuss if GNNs are expressible for FOC2, a fraction of initial order logic. The authors notice that existing GNNs can hardly match the logic. For learning graph topologic structures, Garg et al. (2020) prove that regionally dependent GNN variants do not appear to

be capable to be told world graph properties, at the side of diameters, biggest/smallest cycles, or motifs (Morris et al., 2019).

Loukas (2020) and Dehmamy et al. (2019) argue that existing works exclusively ponder the expressivity once GNNs have infinite layers and units. Shchur et al. (2018) investigates the illustration power of GNNs with finite depth and dimension and discuss the line behaviours of GNNs as a result of the model deepens and model them as dynamic systems.

## Invariance

As there are not any node orders in graphs, the output embeddings of GNNs are imagined to be permutation-invariant or equivariant to the input choices. Maron et al. (2019a) characterize permutation-invariant or equivariant linear layers to form invariant GNNs. Maron et al. (2019b) a lot of prove the result that the universal invariant GNNs square measure typically obtained with higher-order tensorization. Keriven and Peyré (2019) offer another proof and extend this conclusion to the equivariant case. Chen et al. (2019) build connections between permutation-invariance and graph similarity testing. To prove their equivalence, Chen et al. (2019) leverage sigma-algebra to elucidate the expressivity of GNNs (Dehmamy et al., 2019).

## Transferability

A settled characteristic of GNNs is that the parameterization is untied with graphs, that implies the ability to transfer across graphs (so-called transferability) with performance guarantees. (Levie et al., 2019) investigate the interchangeableness of spectral graph filters, showing that such filters are able to transfer on graphs inside identical domain. Ruiz et al. (2020) analyse GNN behaviour on graphons. Graphon refers to the limit of a sequence of graphs, which could even be seen as a generator for dense graphs. The authors conclude that GNNs are transferable across graphs obtained deterministically from the same graphon with wholly totally different sizes (Keriven et al., 2019).

## Label Efficiency

(Semi-) supervised learning for GNNs needs a considerable amount of labelled info to appreciate a satisfying performance. up the label efficiency has been studied inside the attitude of active learning, throughout that informative nodes are actively designated to be labelled by Associate in Nursing oracle to educate the GNNs. Cai et al. (2017) and Gao et al. (2018) demonstrate that by selecting the informative nodes just like the high-degree nodes and unsure nodes, the labelling efficiency square measure typically dramatically improved (Ruiz et al., 2020; Gao et al., 2018).

## CONCLUSION

Predicting student performance is an important issue in current education field of study. However, most current prediction methods treat students individually and do not consider performance correlations between similar students feature. A new pipeline should be proposed for predicting student performance it is based on the newly developed Graph Neural Network. Special, Formalize student grade predictions as

a single student node classification question. A graph consisting of student nodes. To better understand the potential relationships between them as students, we use a variety of similarity learning methods, student's data.

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## Chapter 12

# Methods and Applications of Graph Neural Networks for Fake News Detection Using AI-Inspired Algorithms

**Arpit Jain**

*Koneru Lakshmaiah Education Foundation,  
India*

**Ishta Rani**

*Chandigarh University, India*

**Tarun Singhal**

*Chandigarh Engineering College, India*

**Parveen Kumar**

*Chandigarh University, India*

**Vinay Bhatia**

*Chandigarh Engineering College, India*

**Ankur Singhal**

*Chandigarh Engineering College, India*

### ABSTRACT

*Graph data, which often includes a richness of relational information, are used in a vast variety of instructional puzzles these days. Modelling physics systems, detecting fake news on social media, gaining an understanding of molecular fingerprints, predicting protein interfaces, and categorising illnesses all need graph input models. Reasoning on extracted structures, such as phrase dependency trees and picture scene graphs, is essential research that is necessary for other domains, such as learning from non-structural data such as texts and photos. These types of structures include phrase dependency trees and image scene graphs. Graph reasoning models are used for this kind of investigation. GNNs have the ability to express the dependence of a graph via the use of message forwarding between graph nodes. Graph convolutional networks (GCN), graph attention networks (GAT), and graph recurrent networks (GRN) have all shown improved performance in response to a range of deep learning challenges over the course of the last few years.*

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## INTRODUCTION

Another possible explanation is graph representation learning, which involves the process of understanding how to represent graph nodes, edges, and subgraphs via the use of low-dimensional vectors (Goyal & Ferrara, 2018; Cui et al., 2018a; Hamilton et al., 2017; Zhang et al., 2018a; Cai et al., 2018; Goyal & Ferrara, 2018). Because they depend on hand-engineered features, conventional graph analysis and machine learning approaches are inflexible, time-consuming, and expensive. The SkipGram model is applied to the random walks generated by DeepWalk (Perozzi et al., 2014), which is the first way to graph embedding based on representation learning. DeepWalk was developed by Perozzi and his colleagues. Additionally, substantial progress was achieved in Node2vec, LINE, and TADW. According to Hamilton et al. (2017b), these techniques have two fundamental limitations. First, the encoder does not share any parameters with its offspring nodes. Consequently, the total number of parameters rises proportionately to the total number of nodes, making computation inefficient. Second, direct embedding methods cannot be generalised and cannot handle dynamic graphs.

When creating graph neural networks (GNNs), also known as graph structure data gatherers, CNNs and graph embedding are part of the process. Because of this, they can simulate input and output behaviours that are element-dependent.

The effectiveness of graph neural networks may be evaluated in various ways. In the essay that they published in 2017, Bronstein and his colleagues discuss the problems, prospective solutions, applications, and the future of deep geometric learning. Zhang et al. (2019a) provide a further in-depth analysis and discussion of graph convolutional networks. They explore graph convolution operators, whereas we concentrate on skip connections and pooling operators in GNNs.

The research publications on GNN models carried out by Zhang et al. (2018b), and Chami et al. (2020) are the most current survey studies to be published. Under the findings of Chami et al. (2020), GNNs may be classified as recurrent, convolutional, graph autoencoders or spatial-temporal networks. While Zhang et al. (2018b) provide a comprehensive analysis of graph deep learning approaches, Chami et al. (2020) provide a Graph Encoder-Decoder Model to blend network embedding and graph neural network models. This model was developed in order to improve the accuracy of graph deep learning. This research may be accessed on the web pages maintained by their authors. Our article precisely categorises them and focuses mainly on the more conventional GNN models. In addition, we cover variants of GNN that may be applied to various graphs and their applications in a wide range of business sectors.

In addition, polls were conducted, with the primary emphasis being on learning how to read graphs. An attack on graph data that uses adversarial learning methods and a defence against such an assault. Review of graph attention models. Yang et al. (2020) present learning from a heterogeneous network, which includes multi-type nodes and edges. Huang et al.'s (2020) define the dynamic graph GNN models. Peng et al. (2020) have written combinatorial optimisation graph embeddings are addressed. In Sections 4.2, 4.3, and 8.1.6, the discussion of GNNs for heterogeneous, dynamic, and combinatorial optimisation is ended. The fundamental components of a graph are called nodes and edges. Because of the expressive capability of graphs, they may be used to designate a broad range of systems in the disciplines of social science (social networks; Wu et al., 2020), natural science (physical systems; Sanchez et al., 2018; Battaglia et al., 2016), and knowledge graphs (Yamaguchi et al., 2017). Clustering, link prediction, and node classification are the three critical areas of focus in graph analysis, a non-Euclidean data structure used for machine learning. GNNs are a term used to refer to the deep learning algorithms that work in the graph domain. As a result of the remarkable results it consistently produces, GNN has emerged as

one of the most popular approaches for assessing graphs. Following this, a discussion of the reasons for graph neural networks will occur.

Today's social media channels disseminate hundreds of public and private news items. Accessing material, commenting on posts, and sharing posts on social media should be simple. It is highly suggested that readers remark and share their ideas. However, doing so puts the risk of being exposed to "fake news," which may consist of information that is either false or purposefully manufactured in order to suit political or commercial goals. Because of social media, false information is disseminated more quickly, ultimately, and broadly. Because it is becoming simpler to locate and disseminate false information, fake news presents a risk to the civilisations of the whole globe. In 2017, detecting fake news on social media was a critical study area in academic and professional settings. The efforts made by social media networks to identify websites that disseminate misinformation have been prioritised by such networks. Facebook users are entrusted with fact-checking information and rewarding individuals who report posts that they believe to be misleading or inaccurate. It is possible to boost one's reputation on social media by identifying fake news while it is happening in real-time.

Fake news has the potential to mislead people, which may have adverse effects on both their personal and professional lives. Residents may experience feelings of mental threat or anger due to many fake news articles' efficacy and suggestive nature. This scenario is problematic for communities and cooperative endeavours on three levels: (i) it leads to residents being misinformed; (ii) residents can continue to be misinformed if they live in a media bubble; and (iii) residents can continue to be misinformed if they live in a media bubble. The proliferation of misleading information harmed our economy and our democracy.

In this investigation, GNN is judged against several other machine learning algorithms to determine which are most effective in detecting false news. This study's results help reduce the amount of misinformation shared on social media. When users are provided with access to safe virtual platforms, their experience is simplified. As a component of this research, an analysis of the efficiency of the authenticity detection methods used by GNN will be carried out. It will be much easier to spot rumours and significantly improve the dependability of news posted on social media. Because of this, people's confidence in the various platforms for social media will also deteriorate. Everyone will exercise more caution when it comes to publishing sensitive material. It will also be of use to us in identifying those individuals who spread misleading information.

The investigation of fabricated news has been more popular over the last several years. The topologies of network connections were analysed in this research, which resulted in detecting rumour spreaders, confirming social media rumours, and identifying false news. According to Bovet et al., rumours were the single most important element in the presidential election in the United States in 2016. Xu and his colleagues built a theoretical framework to investigate the expressiveness of GNN in capturing a range of graph topologies and published their findings. The strength of their core design is comparable to that of the Weisfeiler-Lehman graph isomorphism test and the most expressive GNN. When used for social network datasets that include many training graphs, GINs have the greatest amount of success. Benamira et al. suggests combining GNN with a semi-supervised algorithm as a method for data analysis. The fact that they had no hoaxes that could be readily debunked was an issue for them. They concluded that the next step should include semi-supervised learning. Several investigations have shown that the most basic kind of word embedding similarity, based on a nearest-neighbour graph, combined with neural graph networks, may provide highly qualifiable semi-supervised content-based detection approaches. In the research paper that Shivam B. Parikh and his colleagues authored, they developed a method to detect altered and fake tweets across several networks. This dataset offered evidence to support the

conclusions derived from the proposed structure, composed of three basic components. Their method is accurate 83.33 per cent of the time after considering the myriad ways a screen grab from Twitter might be modified. They were questioned by Zhang et al. in search of overt and concealed information. It would be beneficial for their experiment to make use of a Deep Diffusive network illustration. Their experiment determined that their accuracy for multi-class interference was 0.28, while their accuracy for bi-class interference was assessed to be 0.63. It is stated that the accuracy of their hybrid models is 14.5% higher than that of their more traditional equivalents. The approach known as “GDU” can check information simultaneously from several different sources. The study that Tschitschek and colleagues conducted made use of a Bayesian interface. They targeted two distinct types of clients in the end. Because of algorithms, spammers and legitimate users may be distinguished from one another. They employed a Bayesian technique that identifies fake news via the use of crowd signals in order to get past the issue of ambiguity with as little involvement as feasible. Specifically, they wanted to avoid the problem of ambiguity as much as possible. Gangireddy and his colleagues developed a graph-based technique consisting of three parts. It goes by the name GTUT, and it first compiles genuine and fabricated recent news examples. In the second phase, we employ the bi-clique, user, and linguistic similarities that we found before. Last, graph modelling and label spreading label non-bi-clique articles. It helps in accurately recognising each item in the dataset as either false or authentic, depending on the nature of the object. The accuracy of GTUT has increased by more than 10%, while its unsupervised fake news detection accuracy is more than 80%. Shantanu Chandra and his coworkers developed the concept for the social context-aware fake news detection system that would later be known as “SAFER”. They used two distinct datasets to generate their fabricated news: one for celebrity gossip and the other for medical information. Users can publish either fake news or real news, or both. Nguyen et al. conducted research to determine whether or not social environment modelling can be utilised to identify fake news. They proposed a graph learning system that could distinguish ephemeral characteristics that have the potential to differentiate fake news from real news. Their approach minimises the impact of concurrent losses to provide a more comprehensive depiction of social entities.

They assert that the approach is better than others since it avoids the multi-label restriction while concurrently certifying unknown nodes. It is one of the reasons why they believe the method is superior. It is a significant advancement compared to the methods that came before it. The AA HGNN algorithm was developed by Ren and colleagues in order to assess the reliability of various sources of news. The information that they gathered was divided into two categories. Both the schema and node levels are in that order. TextCNN’s performance was much better across the board than those of SVM and LIWC. TextCNN emerged victorious in its battle with LIWC. The highest level of GCN accuracy that they were able to achieve was 0.9688. Curb, created by Kim et al., provides a solution to a one-of-a-kind deterministic optimisation challenge by deciding which bits of news should be fact-checked. Curb was developed by Kim et al. (2020). Their research also finds a relationship between deterministic online optimisation of stochastic differential equations (SDEs), jumps, survival analysis, and Bayesian inference. FakeBERT is the name given to the method created by Kaliyar et al.; it is a deep convolutional technique based on BERT. In order to get optimal results, BERT is combined with three concurrent blocks of 1d-CNN, each of which has a unique kernel size and filter configuration. Their strategy makes use of a BERT that has already undergone training. The accuracy of FakeBERT’s categorisation, which stands at 98.90%, is higher than that of its rivals. While working on MediaEval 2020, Schaal and his associates looked into the 5G Conspiracy and the Corona Virus. Two independent components demand different strategies. They employed a straightforward text-based strategy based on word frequency for the natural language

processing (NLP)-based task that required identification. This method was word frequency-based. When solving issues involving many classes, their GIN model received a score of 0.1810 when it had features and 0.1375 when it did not. Calderbank and colleagues developed the MRF (Markov random field) model by applying the mean-field approach to solve the issue of news validity. Using this method, which involves considering the relationships between several news pieces, it is possible to evaluate the credibility of an article. In the datasets, the unary potential, as well as the paired potential, was calculated.

The importance of spotting fake news and providing potential remedies to the issue has been shown by earlier research based on machine learning. In terms of accuracy, graph neural networks have now achieved a performance level that puts them ahead of their competitors. Node properties of a GNN are user preferences, textual news embedding, and embedded news text, among other things. In most GNNs, the component integration process involves the usage of a news distribution graph. As a consequence of this, we made an effort to investigate and compare several conventional techniques to machine learning and GNN methods.

## **Mathematical Aspects of GNN**

Data is processed via graph neural networks. It accomplishes three tasks. In node classification, node-level tasks anticipate node attributes like labels. For this purpose, the network is frequently split into two groups:  $V_l$  for nodes with labels and  $V_u$  for nodes without labels.  $V_l$  predicts  $V_u$  node properties. Edge-level tasks predict node relationships, such as whether two nodes are connected or edge weights. Graph tasks predict molecular toxicity. Graphs  $G_i$  and labels  $Y_i$  train the model. Unseen distribution graphs are in the test set. GNNs are represented by Equation (1):

$$\varphi = \varphi_0, \varphi_1, \dots, \varphi_n \quad (1)$$

ReLU or sigmoid functions may activate each layer. GNN layers may be graph filters, which modify nodes' hidden representations as in Equation (2)

$$H^{(l+1)} = \sigma(g_l(S, H^{(l)})) \quad (2)$$

Graph pooling layers reduce the graph. Layers that pool obey Equation (3).

$$S^{(l+1)}, H^{(l+1)} = \text{pool}(S^{(l)}, H^{(l)}) \quad (3)$$

$S(l)$  is a filter function that changes the input signal  $H(l)$  while maintaining the graph's structure, represented by  $S$ ; the pool is a function that reduces the graph's node dimension. Most GNNs employ the Message Passing Neural Network (MPNN) framework, including Graph Convolutional Networks (GCN). Spatial GNNs update node representations using neighbour information via aggregation. The AGGREGATE function combines the multiset of neighbours' representations into a single vector, e.g., the sum operator; the UPDATE operator may be a linear mapping of the concatenation of eq(2). UPDATE equals  $h(l) \vee m(l+1) \vee$ . Spectral filters use the Laplacian  $L$  or adjacency  $A$  matrix to update node representations—first, train models on benchmarks. The second strategy guarantees architectural expressiveness theoretically. Measuring GNNs' expressive capacity helps identify tasks they can and

cannot do and compare designs to find more expressive ones. GNNs are exponentially more expressive than MLPs, and tailored for graph-structured data. GNNs build exponentially more rooted graph equivalence classes as their layers advance, unlike MLPs. GNN depth and breadth also impact model expressiveness. If the model is too small or deep, cycle detection, perfect colouring, and the quickest path cannot be recorded. A family of GNNs' capacity to distinguish non-isomorphic graphs or approximate any permutation invariant function on graphs measures its expressiveness.

### **Application of GNN in Various Natures of Problems**

Many graph topologies are large and web-like, making machine learning algorithms difficult to analyse. Studying billion-node social network graphs is tough. Graphs' spatial patterns abstract processing nodes. They are endless nodes. Traditional machine learning vectorises graphs before processing. Preprocessing may disrupt node connections. Graph Neural Networks predict node and edge properties.

Graph Neural Network models emphasise three things:

1. **Node-Focused Tasks.** Regression, categorising nodes, etc. Clustering groups related nodes, whereas classification classifies them.
2. **Edge Chores.** Edge classification and node connection prediction are everyday tasks.
3. **Task Graph.** Predicted and classified graph.

Useful graph neural networks can replicate most events using graph-structured data. Clustering and matching are graph-level issues. Grouping illnesses or molecules is possible—node-level methods like categorisation help. Graph Neural Networks recognise speech, pictures, and text. Deciphering sequences and phrases require text context extraction and recommendation algorithms.

Graph Neural Networks are versatile:

1. User-promotion product partnerships
2. Facebook introductions.
3. Estimating social media or e-commerce interests.
4. Environmental, illness, and viral mutation prediction.
5. Labelling unlabeled data using object labels-based nodes.
6. Processing simulates biological, chemical, and physical systems.
7. Event, place, idea, and entity knowledge graph processing.
8. The user interacts with products, services, and people.
9. Text extraction and sequence labelling.

## **REVIEW OF LITERATURE**

The idea of graph neural networks was the foundation upon which GNNs were built. Recursive Neural Networks were first used to direct acyclic networks in the 1990s (Sperduti & Starita, 1997; Frasconi et al., 1998), but since then, they have been utilised for a variety of other kinds of networks as well.

According to Mikolov et al. (2013), this method uses representation learning and word embedding. Methods on the same level as node2vec, such as LINE and TADW, have also been successful.

The emergence of deep neural networks, most notably convolutional neural networks (CNNs) (LeCun et al., 1998), has breathed fresh life into GNNs and provided them with a second chance at success. CNNs can extract multi-scale, locally-specific spatial information and integrate it into highly expressive world representations.

Both Scarselli et al. (2009) and Micheli (2009) show examples of recurrent and feed-forward neural networks that may be used to manage cycles. Even though effective, these approaches are founded on a fundamental principle that entails iteratively establishing state transition systems on graphs and continuing to do so until convergence occurs. Despite the usefulness of both extendibility and representation, this approach has limitations.

Random walks are performed in Deep Walk (Perozzi et al., 2014), the first method for graph embedding based on representation learning. These random walks are performed by using the Skip Gram model.

According to Hamilton et al. (2017), the use of these methods has two key drawbacks that come along with it. The computing procedure could be more efficient because the encoder's nodes need to communicate their parameters with one another. It is mainly because encoder nodes contribute linearly to an increase in the overall number of parameters. Second, methods that rely on direct embedding cannot deal with dynamic or new graphs because of this limitation. They are obligated to rev up the quality of their outcomes.

Many graph neural networks, also known as GNNs, have been constructed to accumulate data about the structure of graphs. These CNN-based variations use the graph embedding method to accomplish their tasks. As a result, they can represent input and output based on the components themselves and the connections between them.

A few papers focus a considerable amount of emphasis on graph neural networks. Bronstein et al. (2017) examine the problems, possible solutions, applications, and possibilities for the future of deep geometric learning.

The research was done by Goyal and Ferrara (2018). In order to accurately describe network nodes, edges, and subgraphs, low-dimensional vectors should be used (Goyal & Ferrara, 2018; Cui et al., 2018a; Zhang & Cai, 2018a; Hamilton et al., 2017b; Zhang & Cai, 2018a). Traditional approaches to machine learning need hand-engineered characteristics, which renders these approaches rigid, time-consuming, and expensive when applied to graph analysis.

Zhang et al. (2019) investigated convolutional graph networks in depth. While they focus almost all of their emphasis on graph-defined convolution operators, our research focuses on GNN computation modules such as skip connections and pooling operators.

Works by Zhang et al. (2018), Wu et al. (2019), and Chami et al. (2020) are among the most recent publications in the area of GNN survey research. The GNN models are the ones that appear the most often in these studies. Wu et al. (2019) state that GNNs may be classified as recurrent, convolutional, graph autoencoders or spatial-temporal. This information comes from the researchers.

Graph deep learning techniques are investigated by Zhang et al. (2018b), while Chami et al. (2020) provide a Graph Encoder-Decoder Model that integrates network embedding and graph neural network models. Both of the studies may be found at this location. In this investigation, conventional GNN models are used to construct a taxonomy, which is subsequently used to classify the topics. In addition, we talk about the applications of GNN in a broad range of domains and their graph-specific variations. In addition, there have been surveys carried out about the topic of graph education.

Sun et al. (2018) and Chen et al. (2020) address several approaches to graph adversarial learning. Sun et al. (2018) published the first. Among them are assaults on graph data and its defence against them.



An investigation of graph attention models is provided in Lee et al.'s (2018a) work. Learning several representations of heterogeneous graphs is the focus of the study that Yang et al. (2020) conducted. This kind of education comprises nodes and edges, which may assume several distinct appearances. Huang et al. (2020) carried out research that reviewed dynamic graph GNN models.

Peng et al. (2020) provide a condensed explanation of the methods for graph embedding combinatorial optimisation.

## **METHODOLOGICAL APPROACH**

In this part, we go into depth about the techniques for collecting and analysing and applying data.

### **The Origin and Primary Data Source**

We use the dataset from the paper “Fake News,” which consists of text and graph data, to train our GNN models. This dataset provides a variety of information. The actual news material was collected from the FakeNewsNet dataset, which contains the news items and some information on the social activity on Twitter. The information was taken from the FakeNewsNet dataset. The authors of the research, which can be accessed here, collated all of these facts presented here. They crawl all users’ 200 most recent messages using the Twitter develop API to obtain vast historical data. In addition, the URLs supplied in the FakeNewsNet dataset are used to analyse the news content. To incorporate it into our text-based classification models, we build a crawler to extract all the news data from the URLs supplied in the FakeNewsNet dataset. The information fact-checked by Politifact and gossip cop indicates that the dataset includes false and factual news and dissemination statistics for each story.

### **Processing the Data**

Raw text data that has yet to be processed in any way often contains mistakes, inaccuracies, and inappropriate information. The data should be preprocessed as a problem-solving method, seeing as how this approach has been successful in the past when used in similar situations. After crawling all accessible news stories, the first stage in our data processing is to strip the text contents of any non-alpha data and special characters. It happens after we have completed the crawling process. In addition to this, we get rid of any potential ending words that may have been there. After that, we use the NLTK online tokeniser to tokenise the remaining text streams into a glossary of words. In addition, we use a Count vectoriser to transform the numerical data produced by the input text. A test and train data set were derived from the corpus and used in the training process. Eighty per cent of the data set is made up of the test data, while the remaining twenty per cent is made up of the train data. It contains the data we pull from the paper’s news propagation graph for usage in our GNN models. These are the data that we employ. They used the method described in and into practice to build the graph representing how information spreads. They take advantage of the timestamps supplied by users when they publish or repost a specific piece of news to generate the propagation graph for that particular piece of news. They incorporate both the news content and the prior posts made by active users using text representation learning methods such as Word2vec and BERT. In addition, they employ spaCy for the pre-trained word2vec vector, which is made up of pre-trained vectors with a total dimension of between 300 and 685k.

## Procedures That Were Carried Out

This chapter will discuss each component that makes up our models. We put two separate classification algorithms into place: text-only data and text-only data and graph data, as shown in Table 1 and Table 2.

*Table 1. Primary data fetching through the URLs*

Datasets	Politifact	Gossip Cop
Fake News	2500	7500
Real News	3000	7000
Total	5500	14500

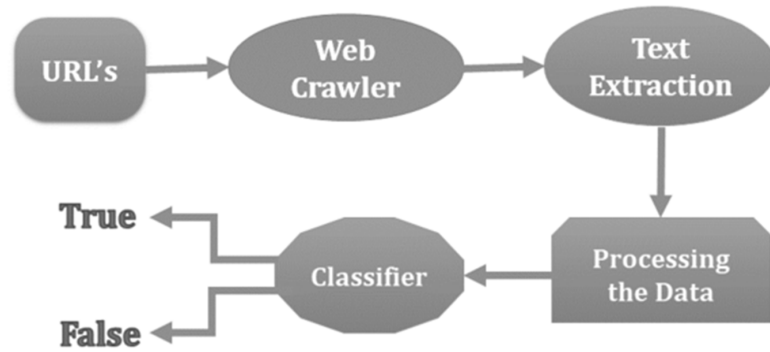
*Table 2. Primary data of graph for graph neural network models*

Datasets	Gossip Cop	Politifact
Graphs	5896	216
Fake News	3033	181
Total Nodes	354,000	38954
Total Edges	325632	42546
Avg. Nodes per Graph	55	140

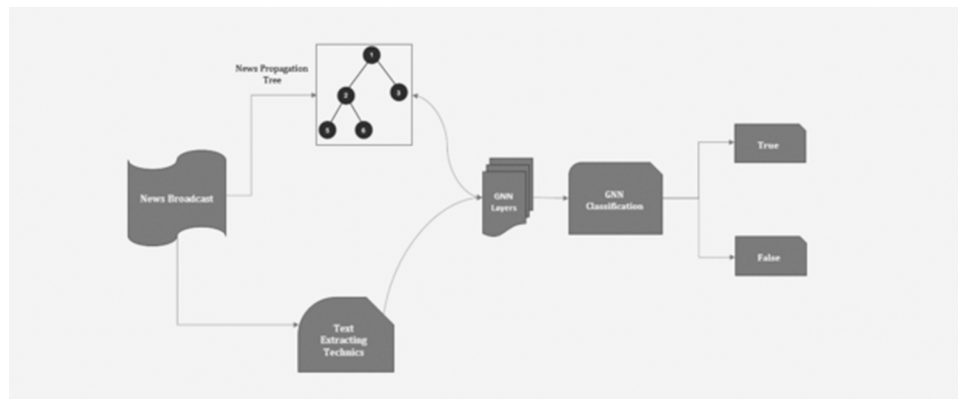
Because it is one of the supervised machine learning approaches that may be used to solve a wide range of classification issues, the Support Vector Machine (SVM) is the method we employ for our text-based classification. It is the case for the simple graphical model (SVM), one of the approaches discussed. In addition to this, we make use of decision trees, random forests, and logistic regression. The decision tree and the logistic regression model can analyse categorical data. Due to its unique algorithm, Random Forest also excels at categorising. Forest (RF) was shown to generate the highest accurate results after an experimental study of 179 different classifiers applied to 121 unique datasets by Fernandez- Delgado et al. Text-based classifications workflow is shown in Figure 1.

Alternately, to generate reliable predictions based on text and graph data, we use GNN models with many convolutional layers. The “message passing neural network” strategy introduced by Gilmer et al. is one we use in the classification models based on text and graphs we have developed. The GNN developed this mechanism. The message transmission process involves the whole graph neural network at every layer. Each node in the graph is responsible for carrying out the following operations: (1) It gathers the representations of all the other nodes that are immediately next to it; (2) It carries out an aggregation operation; and (3) It updates the representation of its node. Classification Workflow through Text and Graph is shown in the graph.

*Figure 1. Classifications workflow based on fetched text data*



*Figure 2. Classification workflow through text and graph*



## RESULTS AND ANALYSIS

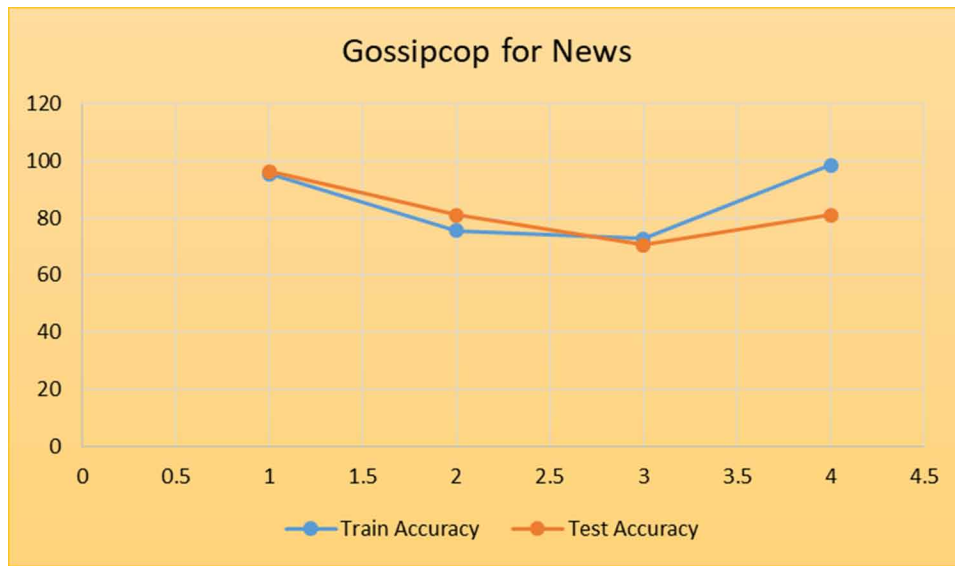
Throughout our analysis, we used two separate datasets from Gossipcop and Politifact. The three basic categories of node attributes learnt via the application of text representation learning techniques are shown in each dataset. The 768-dimensional Bert approach, the 300-dimensional spacy method, and the 10-dimensional profile method are also examples of alternatives. The Spacy and BERT techniques encode the user's endogenous preferences in this scenario, while the Profile method serves as a baseline for comparison. In order to identify instances of false news, we used many different iterations of the GNN algorithm, including GAT, GraphSAGE, GCN, and GIN. A comparison of Supervised Learning and GNN Variants in Detecting Fake News is shown in Table 3.

The graphs in Figures 3-6 show the training accuracy vs test accuracy over the number of epochs plotted in the following snippets.

Table 3. Comparison of supervised learning and GNN variants on detecting fake news.

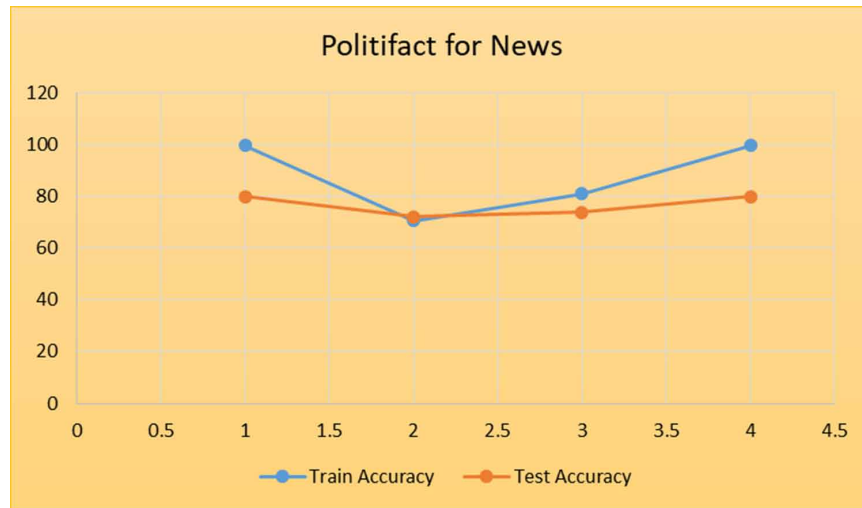
Mode	Model	Gossip Cop		Politifact	
		Train Accuracy	Test Accuracy	Train Accuracy	Test Accuracy
News Only	Logistic Regression	95.32	96.36	99.68	80
	SVM	75.65	80.93	70.62	72
	Decision Tree	72.65	70.62	80.93	73.75
	Random Forest	98.51	80.93	99.68	80
News + Graph	GAT	100	78.36	99	93.6
	GraphSAGE	100	98.9	99	93.6
	GCN	99.18	96.84	99	93.6
	GIN	98.35	93.05	99	93.6

Figure 3. Training accuracy vs test accuracy over the Gossipcop for news

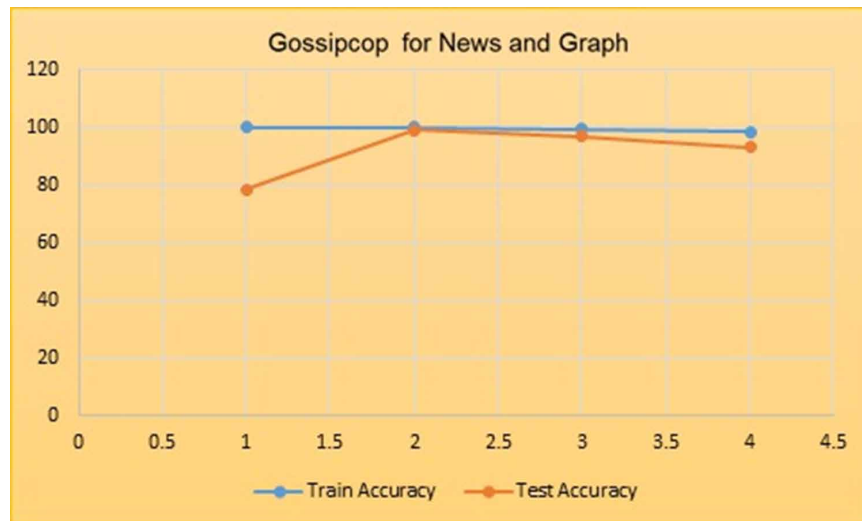


Roughly a hundred epochs were run for each method to train, verify the accuracy level, and quantify the loss function. It was done in order to train and validate the technique. All versions of GNN were updated when this was finished. Table 3 compares the performance of four different Supervised Learning algorithms (Logistic regression, SVM, Decision Tree, and Random Forest) and four distinct GNN versions (GAT, GraphSAGE, GCN, and GIN) in terms of their capacity to identify fake news. Compared to the performance of other Supervised Learning algorithms, each of the four unique GNN versions achieves higher success. On the datasets from Gossipcop, GNN variants exceeded the best-Supervised Learning algorithms (Logistic regression and Random forest) by 15–18%, whereas on the datasets from Politifact, GNN variants only outperformed the best-Supervised Learning algorithms by 4%. On the Gossipcop datasets, GNN variants outperformed the best-Supervised Learning algorithms by 15–18%.

*Figure 4. Training accuracy vs test accuracy over the Politifact for news*

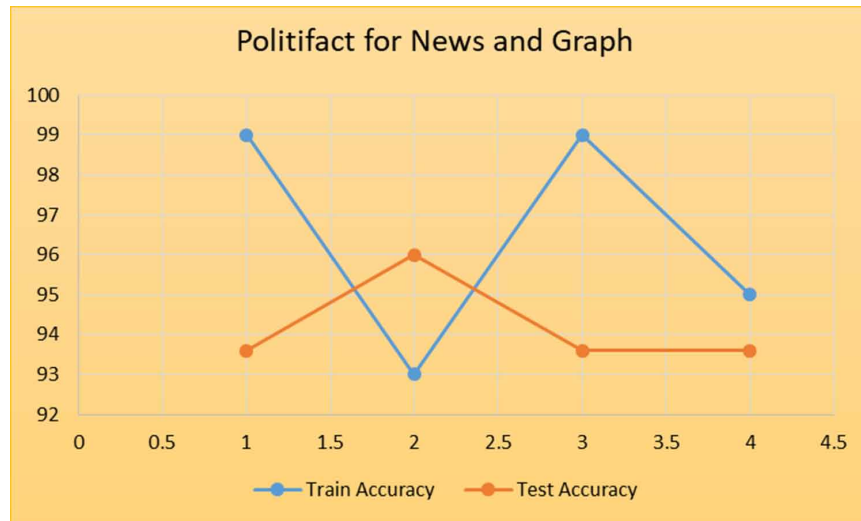


*Figure 5. Training accuracy vs test accuracy over the Gossipcop for news and graph*



Second, supervised learning algorithms were exclusively applied to the news content, whereas versions of GNN were applied to both the news content and the propagation graph. It was done in order to understand the relationship between the two better. When we use data from visuals and the news, it is evident that we can achieve a greater degree of accuracy than when we depend exclusively on news items. Table 3 of the Gossipcop dataset demonstrates that GraphSAGE has a more considerable accuracy of 96.99% for the 768-dimensional Bert approach and 96.52% for the 300-dimensional spacy technique, whilst GAT has a greater accuracy of 93.27% for the 10-dimensional profile technique. Both of these results can be found in the table. These figures were calculated based on GraphSAGE’s overall performance.

Figure 6. Training accuracy vs test accuracy over the Politifact for news and graph



In comparison, the 768-dimensional Bert method achieves a greater accuracy of 85.07% in the Politifact dataset. The 10-dimensional profile technique surpasses the GraphSAGE model by 78.28%, and the 300-dimensional spacy strategy exceeds the GCN model by 82.82%. Both of these techniques outperform the GCN model. The same results are obtained by GIN when using the 768-dimensional Bert technique. It is important to note that the endogenous approaches (Bert and Spacy) that keep user profile data tend to perform better than the profile feature, which is the case for both datasets. It is something that should be taken into consideration. In addition, we found that GraphSAGE and GCN had the most outstanding overall performance compared to the other models. It was the conclusion we came to after analysing all analysing data. The sections of Figure 3 are excerpts from that figure, which compare the training data's accuracy to the test data's accuracy as a function of the number of epochs ( $n$ ). Figure 3 contains several graphics that provide the most precise illustration of the accuracy of the comparisons made between our models' Train and Test versions. The orange curve in these pictures shows the accuracy of the test, whereas the blue curve shows the accuracy of the train. In light of the information shown in these graphs, we can draw the following conclusion: the precision of the train has a minor influence on the correctness of the test.

## CONCLUSION AND FUTURE SCOPE

The purpose of this research was to investigate the viability of using GNN as part of the process of evaluating the credibility of news stories. In order to battle one of the most severe problems that our contemporary, socialised so socialised ronts, namely the spotting of false news, GNN can provide a hand when it is required to do so. We used a dataset called UPFD, which was then integrated with specific programmes called Pytorch Geometric (PyG) and Deep Graph Library (DGL). In the future, additional data from other social media platforms, such as Facebook and Instagram, will be able to be gathered and compared to examine the distribution patterns of actual vs false news. It will allow for a more in-depth

examination of the issue. It will be helpful to discover which platform the information transfer affects to determine which social media network a person or community uses. We need a particular dataset; we may develop a technique to produce this data from regular text datasets. If we are successful, this would be a significant step forward. In this instance, we used a dataset written in English; however, in the future, we may use datasets written in other languages. A second area that might benefit from future contributions is the creation of real-time applications in datasets to assist in the battle against false news. It is essential to find a solution to this problem.

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## **KEY TERMS AND DEFINITIONS**

**GCN:** A GCN is a variant of a convolutional neural network that takes two inputs.

**GNN:** Graph Neural Network (GNN) comes under the family of Neural Networks which operates on the Graph structure and makes the complex graph data easy to understand.

## Chapter 13

# Comprehensive Study of Face Recognition Using Feature Extraction and Fusion Face Technique

**Jayanti Mehra**

*Lakshmi Narain College of Technology, Bhopal, India*

**Neelu Singh**

*Lakshmi Narain College of Technology, Bhopal, India*

### ABSTRACT

*Face recognition is a process by which the identity of a person is determined from the face images stored in a face database. Face recognition is one of the most successful applications of image analysis. In the present scenario, face recognition plays a major role in commercial and law enforcement applications, such as surveillance system, passport, security, personal information accesses, human machine interaction, etc. At present, very reliable methods of biometric personal identification exist. In face recognition, a feature vector usually represents the salient characteristics that best describe a face image. However, these characteristics vary quite substantially while looking into a face image from different directions. This chapter addresses this issue by means of image fusion and presents a comprehensive study of different image fusion techniques for face recognition. Image fusion is done between the original captured image and its true/partial diagonal images.*

### INTRODUCTION

Face recognition is a process by which the identity of a person is determined from the face images stored in a face database (Dey et al., 2014). Face recognition is one of the most successful applications of image analysis. In present scenario, face recognition plays a major role in commercial and law enforcement applications, such as, surveillance system, passport, security, personal information accesses, human

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machine interaction, etc. (Yuille et al., 1989; Zitová et al., 2003). At present, very reliable methods of biometric personal identification exist. The fingerprint analysis, retinal or iris scans, etc., are examples of the biometric personal identification method. However, these methods rely on the active cooperation of the participants (Graham et al., 1998). The person identification system, which is based on analysis of frontal or profile images of the face, is very effective without the participant's cooperation or knowledge. Face perception is an important part of the capability of human perception system (Alvarado et al., 2006). It is also a routine task for human. It is a true challenge to build a computer system which parallels human ability to recognize faces. Therefore, face recognition has become an active research area, and it attracts researchers from the field of image processing, pattern recognition, neural networks, computer vision, etc. (Zhou et al., 2014). Although, presently the face recognition system has reached a certain level of maturity, but the success of the face recognition system is limited by the conditions imposed by many real-world applications. For example, face recognition in an outdoor environment with variations in illumination, and/or pose remains a very challenging problem (Fraser et al., 1998; Sing 2015). Therefore, the present systems are still far away from the capability of the human perception system. The face recognition system can be developed as a three-step process (Li, 2014). The first step of the face recognition system is face detection (Keller et al., 1985). Face detection is the process of extracting face region from the input scene (Yang et al., 2004). It has many applications in face tracking (Zhuang & Dai, 2007), pose estimation, compression, human-computer-interaction (HCI) system, etc. The next step of the face recognition system is feature extraction (Tan et al., 2006), which acquires relevant facial features from the face images (Adini et al., 1997; Zou et al., 2007). Features are properties which describe the whole face image (Xu et al., 2013). Feature extraction process must be efficient enough in terms of computing time and memory usage (Kwak et al., 2005). There are many applications of the feature extraction process in facial feature tracking, emotion recognition, gaze estimation, and human-computer-interaction (HCI) system (Nandakumar 2008; Cament et al., 2015; Shen et al., 2004). The face detection and feature extraction are often performed simultaneously (Er et al., 2002; Bartlet et al., 2002). The final step is face recognition. In this phase, the face images are identified or verified by applying the extracted facial features on some classifiers (Zhao et al., 2012).

## **PROCEDURE TO GENERATE THE DIAGONAL IMAGES**

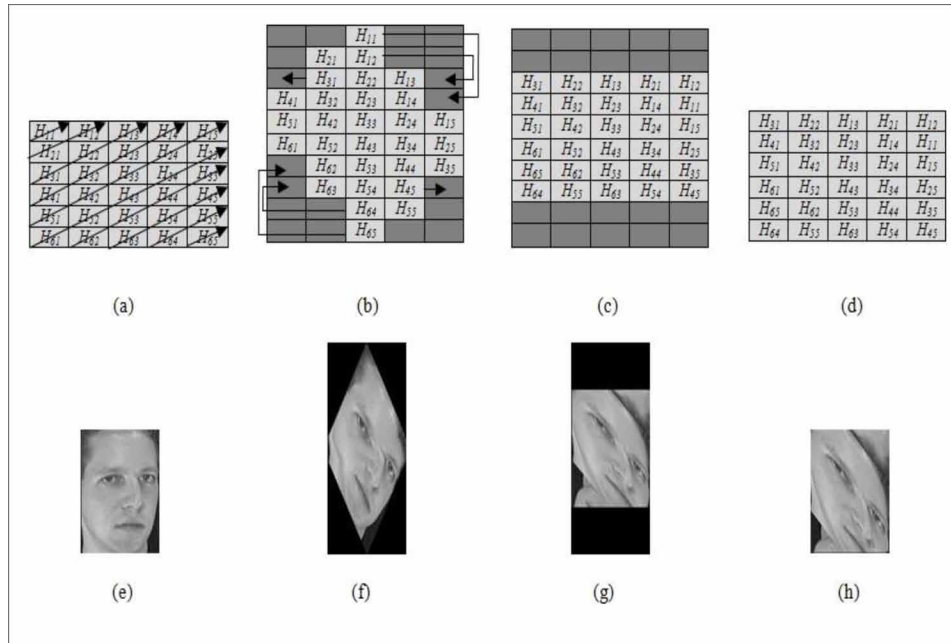
### **Generation of true diagonal images**

Let  $X$  be an image matrix of dimension  $m \times n$  as shown in Figure 1(a). We start to scan the image matrix from the upper left-corner pixel, along the diagonals from left to right upwards, towards the lower right-corner pixel. Pixel(s) of the major and minor diagonals are placed into rows of the diagonal image starting from the top row, ensuring that the pixel(s) of the minor diagonals are placed in the middle of the corresponding row as shown in Figure 1(b). The generated diagonal image may be either square (if  $m=n$ ) or rectangle (if  $m \neq n$ ) in size. Thus, we generate true diagonal images from the original face images by placing the diagonal vectors along the horizontal direction. As a result, its size is greater than the original one. The dimension of resultant truly diagonal image is  $(m + n - 1) \times \text{MIN}(m, n)$ . Since, the size of the diagonal image matrix is higher; this diagonal face images are scaled down into the size of the original face images( $m \times n$ ).

## Generation of Horizontal Partial Diagonal Images

To make the resultant diagonal image same in the size that of the original image, the top most single pixel as well as bottom most single pixel shifted into the nearest row where the maximum number of blank pixel is one. Then we shift the next top most two pixels as well as next bottom of two pixels into the nearest row where the maximum Number of blank pixels is two. This process is repeated until all the pixels of the diagonal image matrix come to a shape of dimension  $m \times n$ , as shown in Figures 1(b), 1(c), and 1(g). However, due to this process, the continuities of some of the image pixels are broken and thereby we call it as a horizontal partial diagonal image. The final resultant horizontal partial diagonal image matrices are shown in Figures 1(d) and 1(h).

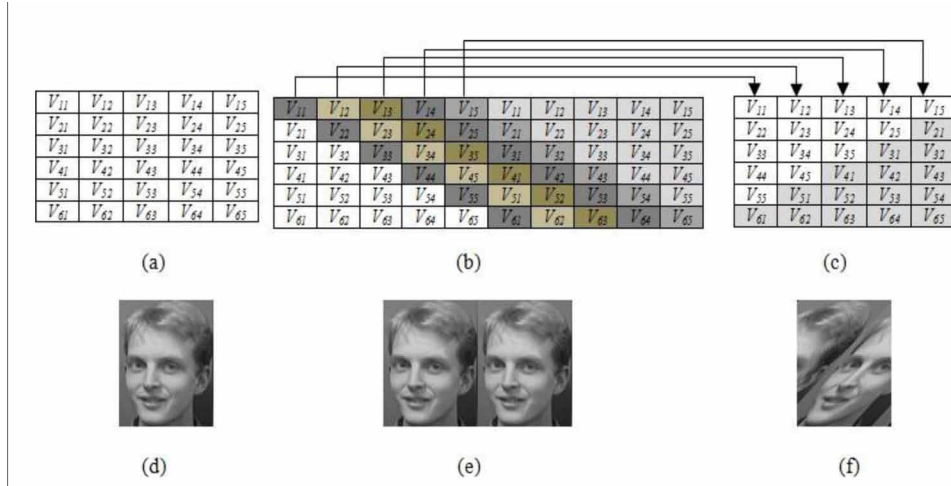
Figure 1. Generation of horizontal partial diagonal image: (a) and (e): original images; (b) and (f): truly diagonal images; (c) and (g): intermediate images; (d) and (h): horizontal partial diagonal images



## Generation of Vertical Partial Diagonal Images

To produce vertical partial diagonal image matrix, at first, we append two same face image matrices just one after another side by side as shown in Figure 2(e). Let the size of original image matrix (shown in Figure 2(a) and (d)) is  $m \times n$ . Therefore, the size of the fused image matrix will be  $m \times 2n$  (shown in Figure 2(b) and 2(e)). Now we start the scanning process from top most left corner pixel and move diagonally from the left to right own ward sand put these pixel(s) along the column of a matrix, as shown in Figure 2(b) and 2(c). The process is repeated for  $n$  times producing the final image of size  $m \times n$  as shown in Figure 2(c) and 2(f). Like the previous one, here also the continuities of some of the image pixels are broken and thereby we call it as a vertical partial diagonal image.

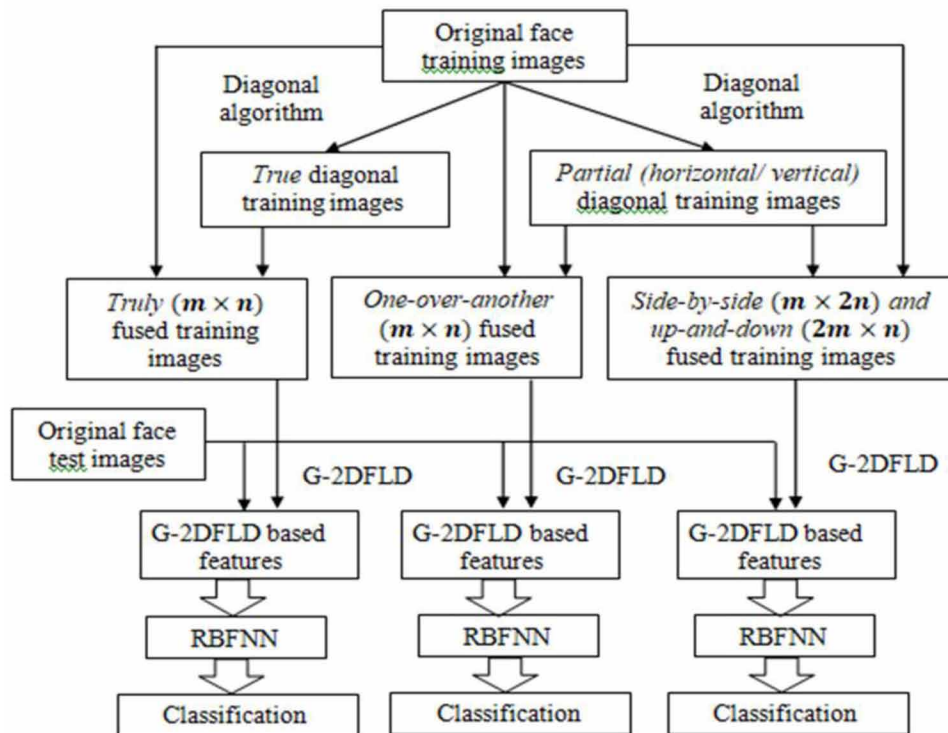
Figure 2. Generation of vertical partial diagonal image: (a) and (d): original images; (b) and (e): intermediate images; (c) and (f): vertical partial diagonal images



## Problem Definition and Image Fusion Techniques

The idea behind is that the human cognition process can recognize a face by looking in to the horizontal, vertical and also diagonal vectors of the image matrix.

Figure 3. Schematic diagram of proposed method



To exploit this, in this Section, we propose three image fusion techniques between the original and three diagonal (true and partial) images. Figure 3 shows the schematic diagram of the proposed method. All training images are diagonalized to generate their true and partial diagonal images. The original and diagonal images are fused in the forms of (i) one-over-another using original and true diagonal images and (ii) one-over-another using original and partial diagonal images and (iii) side-by-side and up-and-down using original and partial diagonal images. We have used the generalized 2-dimensional Fisher's linear discriminant (G-2DFLD) (N. Zheng et al., 2014) method for feature extraction from these fused images. Finally, a radial basis function (RBF) neural network is used for classification and recognition.

### **Fusion of Original Image With Its True Diagonal Image as One Over Another**

In this method, we fuse the original and its true diagonal image as one-over-another (superimposed) as shown in Figure 4. The objective is to get the texture information from both the original and diagonal images at the same time. However, due to this process, pixel intensity values may exceed beyond the permissible limit; there by reducing the contrast of the fused image. For proper further analysis, we need to enhance its contrast.

#### **Contrast Enhancement**

Let  $min$  be the minimum pixel value of the fused image matrix  $XS$ . Now, subtract  $min$  from each pixel of the  $XS$ . After this operation, let  $max$  is the maximum pixel value of the  $XS$  image matrix. We define an enhancement factor (EF) as follows:

$$Enhancement\ Factor(EF) = max / maximum\ gray\ scale\ value \quad (1)$$

Now, each pixel value of the  $XS$  image matrix is updated by dividing with the enhancement factor (EF). Then  $XS$  values are defined as follows:

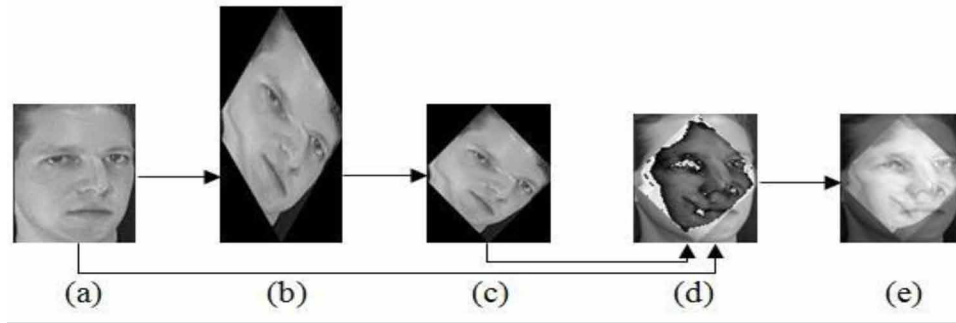
$$XS = XS / EF \quad (2)$$

The resultant image by the Eq. (1.2) gives the contrast enhanced fused image matrix, as shown in Figure 4(e).

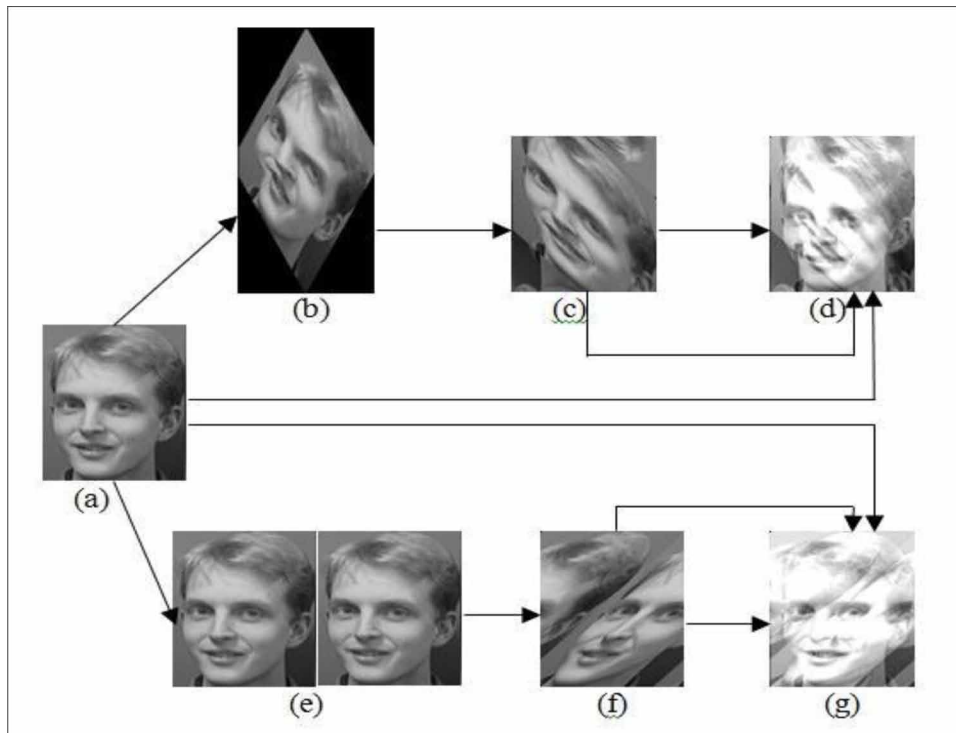
### **Fusion of Original Image With Its Partial (Horizontal and Vertical) Diagonal Image as One Over Another**

The original image is fused with the horizontal partial diagonal image as well as vertical partial diagonal image. The different steps are illustrated in Figure 5.

*Figure 4. Generation of superimposed fused image: (a): original image; (b): true diagonal image; (c): resized the true diagonal image into the size of original image; (d): resultant superimposed fused image; (e): resultant contrast enhanced superimposed fused image*



*Figure 5. Generation of superimposed image: (a): original image; (b) and (e): intermediate images; (c) and (d): horizontal partial diagonal image and super imposed image, respectively; (f) and (g): vertical partial diagonal image and super imposed image, respectively*

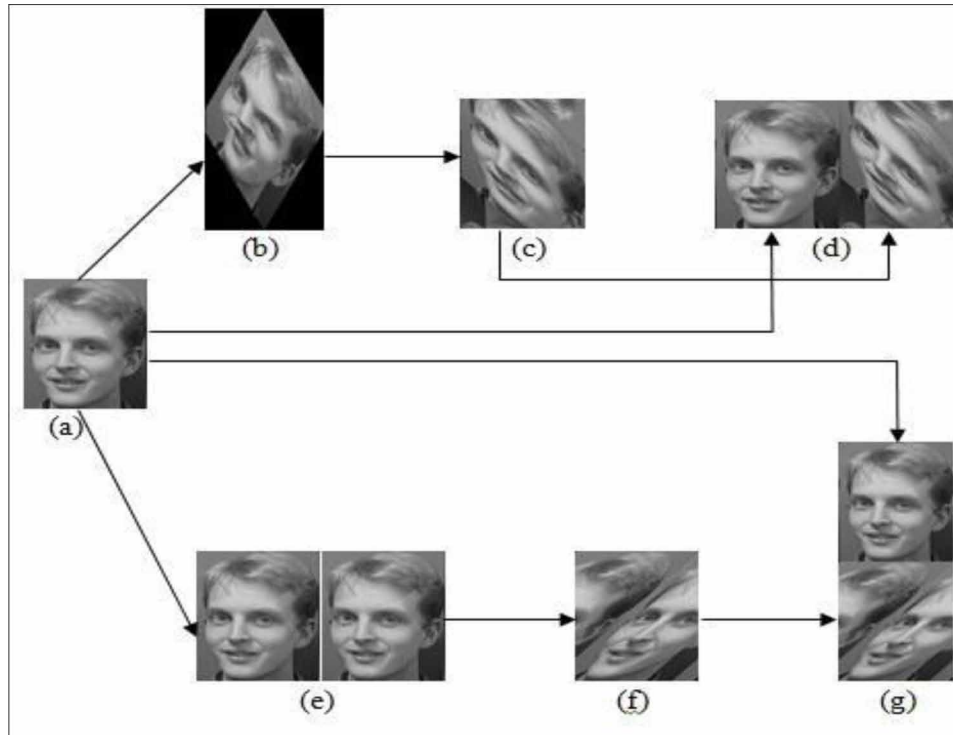


### **Fusion of Original Image With Its Partial (Horizontal and Vertical) Diagonal Image as Side-by-Side and Up-and-Down**

The objective is to get the textural information from the original and partial diagonal images one after another. To realize this, the horizontal partial diagonal face image matrix is appended at the right side

of the original image matrix. Similarly, the vertical partial diagonal face image matrix is appended at the bottom of the original image matrix, as presented in Figure 6. This process actually augments the information available with the original image with that of the partial diagonal image. The dimensions of horizontally and vertically fused face image are  $m \times 2n$  and  $2m \times n$ , respectively.

Figure 6. Generation of horizontally and vertically fused image: (a): original image; (b) and (e): intermediate image; (c) and (d): horizontal partial diagonal image and horizontally fused image; (f) and (g): vertical partial diagonal image and vertically fused image, respectively



## DISCRIMINANT OF EXTRACTION FEATURE FROM FUSED IMAGES

In case of designing face recognition systems, one needs to extract a set of discriminative features from the face images, which in collectively differ from person (class) to person. In particular, these features should yield most dissimilar score among the images of two different persons and similar or identical score for the same person.

Since the objective is to extract features from both the original and diagonal images at the same time, we have suitably modified the generalized two-dimensional Fisher's linear discriminant (G-2DFLD) method (Zheng et al., 2014) to work with the fused images. The G-2DFLD method is proven to be superior to other holistic-based feature extraction methods and extracts features in the directional information in an image. The extracted features increase discrepancy between classes and coherency within classes. The G-2DFLD method can be directly used on the superimposed fused images for feature extraction, in cases of horizontal and vertical fused images, we have modified it as stated below:



## Comprehensive Study of Face Recognition

Let, the training set consist of N number of training face images of C distinct persons, where each face image is of  $m \times n$  dimension. Therefore, the horizontal  $Xh$  and vertical  $Xv$  fused images will be of dimensions  $(m \times 2n)$  and  $(2m \times n)$ , respectively.

Step 1: Compute the  $rh$  and  $rv$  as the mean images of the horizontal and vertical fused images, respectively. Further, compute  $hc$  and  $vc$  as the mean images of the  $c$ th person corresponding to horizontal and vertical fused images, respectively.

Step 2: Compute the between-class and within-class scatter matrices ( $Shb, Shw$ ) from the horizontal fused images. Similarly compute ( $Svb, Svw$ ) scatter matrices from the vertical fused images. They are computed as follows:

$$S_{hb} = \frac{1}{N} \sum_c^C N_c (\tau_{hc} - \tau_h) (\tau_{hc} - \tau_h)^\tau \quad (3)$$

$$S_{hw} = \frac{1}{N} \sum_c^C \sum_{i \in c}^N (X_{hi} - \tau_{hc}) (X_{hi} - \tau_{hc})^T \quad (4)$$

$$S_{vb} = \frac{1}{N} \sum_c^C N_c (\tau_{vc} - \tau_v) (\tau_{vc} - \tau_v)^\tau \quad (5)$$

$$S_{vw} = \frac{1}{N} \sum_c^C \sum_{i \in c}^N (X_{vi} - \tau_{vc}) (X_{vi} - \tau_{vc})^\tau \quad (6)$$

Where  $N_c$ ,  $X_{hi}$  and  $X_{vi}$  are the number of images in class  $c$ ,  $i$ th image of the horizontal and vertical fused images, respectively.

Step 3: Define the two Fisher's criteria  $J(P)$  and  $J(O)$  to derive the **projection** matrices as follows:

$$J(P) = \arg \max_P |P^T S_{hb} P| / |P^T S_{hw} P| \quad (7)$$

$$J(O) = \arg \max_Q \frac{|O^T S_{vb} O|}{|O^T S_{vw} O|} \quad (8)$$

Step 4: Obtain the optimal projection (eigenvector) matrices  $P_o$  and  $O_o$  by solving the following equations:

$$P_o = \arg \max_P \left| S_{hb}^{-1} \right|_{P^T} h w \quad (9)$$

$$O_o = \arg \max_Q \left| S_{vb}^{-1} \right|_{Q^T} v b \quad (10)$$

Step 5: Extract feature vector  $F$  for an image  $X$  by the following equation:

$$F = PoTXOo \quad (11)$$

## CLASSIFICATION USING RADIAL BASIS FUNCTION NEURAL NETWORK

After feature extraction, we need to classify and recognize the images based on their extracted features. In this work, we have used a radial basis function neural network (RBFNN) for classifying the image due to its simple structure and faster learning ability (Chowdhury et al., 2011).

Determine the class of the  $i$ th pattern  $f_i$  as the index of the output neuron, which produces maximum value as stated below:

$$class(f_i) = \arg \max_{k=1,2,3,\dots,C} (z_{ik}) \quad (12)$$

## EXPERIMENTAL RESULTS

The performance of the present method has been evaluated on the AT&T Laboratories Cambridge face database (Phillips 2007), the UMIST face database (Phillips et al., 2000), and the FERET face database (The ORL face database) (Chowdhury et al., 2011) using an IBM Intel I5 Hyper-Threading technology, 3.0 GHz, 8 GBDDR-III RAM computer running on Fedora 18 Linux Operating System.. We have done many experiments by considering different configurations of the present method to test its performance (Belhumeur et al., 1997). Finally, the average recognition rate  $R_{avg}$  has been calculated with the help of the equation (2). The method (denoted  $d_{as}$  m1) where true diagonal image is super imposed with original one yields superior results than the other two methods m2(where, partial diagonal image is placed horizontally and vertically with the original one) and m3 (where, partial diagonal image is superimposed with the original one). In our experiments, the radial basic function neural network (RBFNN) classifier has been used for training, classification and recognition.

### Experiments on the AT&T Face Database

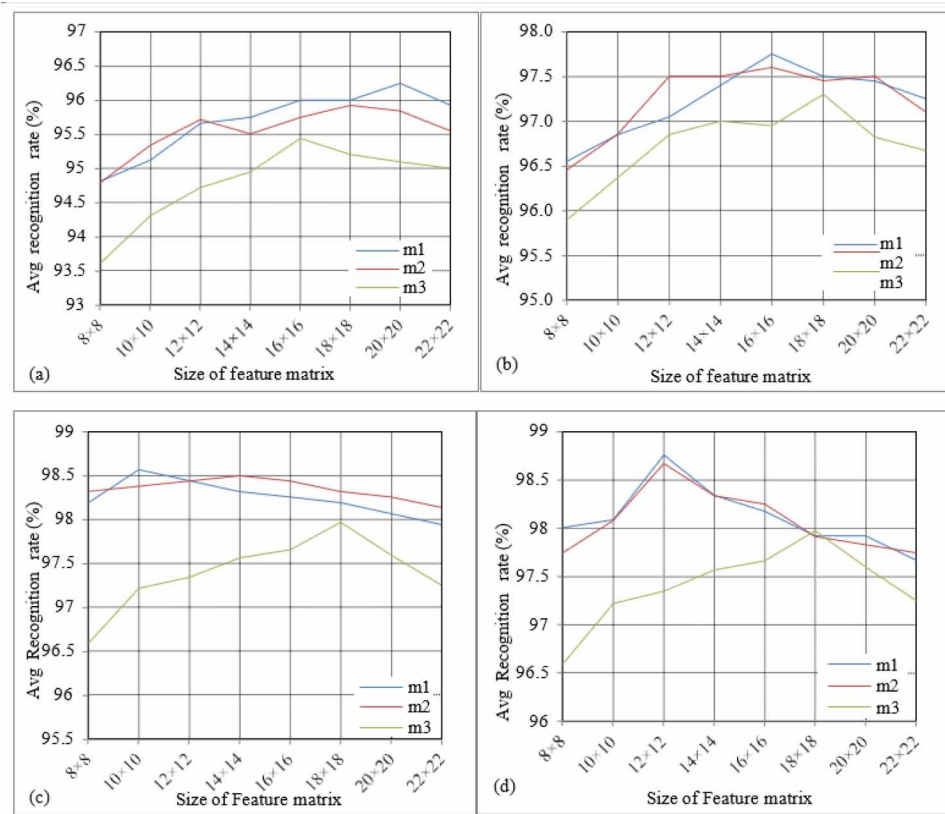
In this Section, we discuss the performance of the present method on the AT&T face database. In this experimental strategy, the AT&T face database (Chellappa et al., 1995) is randomly partitioned into training and test sets. Figure 7 describes a comparative analysis of the three fusion methods on the AT&T face database (Huang, 1998). The analysis is done by varying feature size from  $8 \times 8$  to  $22 \times 22$  in terms of average recognition rates in 20 experimental runs with different training and test sets. A training set is generated by pickings images/person (here,  $s=4,5,6$  and  $7$ ) randomly and placing the remaining images into the test set. The m1 method has the highest average recognition rates of 96.25% ( $20 \times 20$ ), 97.75% ( $16 \times 16$ ), 98.56% ( $10 \times 10$ ), and 98.75% ( $12 \times 12$ ), respectively with 4, 5, 6, and 7 training images/class, respectively.

The RBFNN is modeled with 120, 120, 160 and 160 hidden layer nodes for 4, 5, 6, and 7 training samples per person, respectively.

## Comprehensive Study of Face Recognition

For fair of comparison, the performance of the three fusion methods discussed in the previous Section are compared with other holistic-based approaches (G-2DFLD, G-Dia2DFLD, Dia FLD, and 2DFLD) methods on the AT&T face database. From experimental results it can be concluded that, the present method is efficient than other methods in terms of total computation time (Chowdhury et al., 2011). The comparisons of these approaches along with the present three fusion methods method in terms of best average recognition rates(%)by randomly partitioning the AT&T face database are summarized in Table 1. In all of these experiments, we have used the same radial basis function (RBF) neural network and parameters for training, classification and recognition.

Figure 7. Comparative study of average recognition rates (%) on the AT&T database for different values of  $s$  by varying feature size: (a)  $s=4$ , (b)  $s=5$ , (c)  $s=6$ , (d)  $s=7$



Simulation results demonstrate that in all the cases, the performances of the present method are better than other (four) methods. The tabulated results illustrate that the m1 method outperforms the other methods in all experimental runs. This indicates that by using the information both from original and true diagonal images together, it is possible to extract superior discriminative features. The recognition rate increases with the size of the feature matrix whenever the discriminant feature value is high (Kumar et al., 2022).

Table 1. Comparison with the to her methods in terms of average recognition rate on the AT&T database (figures within the parentheses denote the size of features)

Method	Averagerecognitionrates			
	$s=4$	$s=5$	$s=6$	$s=7$
True diagonal image superimposed with original image(m1)	<b>96.25</b> (20×20)	<b>97.75</b> (16×16)	<b>98.56</b> (10×10)	<b>98.75</b> (12×12)
Partialdiagonalimage placedhorizontaland verticalwithoriginal image(m2)	95.92 (18×18)	97.6 (16×16)	98.5 (14×14)	98.67 (12×12)
Partialdiagonalimagesu perimposed withoriginalimage (m3)	95.44 (16×16)	97.3 (18×18)	97.97 (18×18)	97.83 (18×18)
G2DFLD	95.94 (16×16)	97.68 (14×14)	98.72 (14×14)	98.42 (8×8)
G-Dia2DFLD	93.27 (19×13)	95.05 (19×26)	96.48 (26×24)	97.13 (17×23)
DiaFLD	92.73 (112×5)	94.88 (112×5)	96.31 (112×5)	96.71 (112×35)
2DFLD	95.08 (112×16)	97.50 (112×14)	98.26 (112×14)	97.88 (112×8)

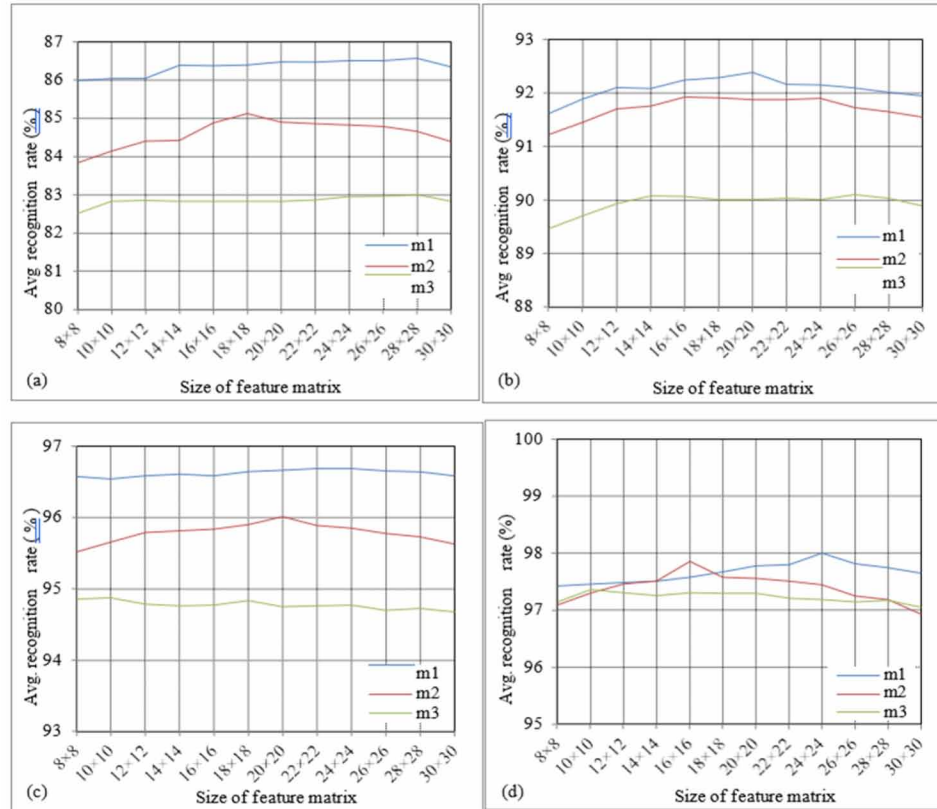
## Experiments on the UMIST Face Database

In this Section, the performance of the present method on the UMIST face database is discussed. In this face database, the performance of three proposed fusion method has been evaluated in this Section. In this experimental strategy, the database is partitioned randomly into training and test sets. For each and every values of  $s$ , we have repeated the experiment 20 times with different training and test sets. The investigation is done by varying feature size from  $8 \times 8$  to  $30 \times 30$  in terms of average recognition rates in 20 experimental runs with different training and test sets. For  $s=4, 6, 8$  and  $10$ , the m1 method achieves best average recognition rates 86.56% ( $28 \times 28$ ), 92.37% ( $20 \times 20$ ), 96.7% ( $22 \times 22$ ) and 98.02% ( $24 \times 24$ ), respectively. The RBFNN is modeled with 60, 100, 140, and 180 hidden layer nodes for 4, 6, 8, and 10 training samples per person, respectively.

The performance of the three fusion present methods has been compared with the G-2DFLD, 2DFLD, 2DPCA, PCA+FLD, and PCA approaches on the UMIST face database. The comparisons in terms of best average recognition rates (%) of these methods along with the present method by randomly partitioning the UMIST face database are shown in Table 2. The same radial basis function (RBF) neural network and parameters are used for training, class if I action and recognition in all of these experiments. From experimental results in the table, it can be observed that in all the cases, the performances of the method m1 method out performs to that of the G-2DFLD, 2DFLD, 2DPCA, PCA+FLD, and PCA methods,

in terms of recognition rate. This indicates that by using the information both from original and true diagonal images together, it is possible to extract superior discriminative features.

Figure 8. Comparative study of average recognition rates (%) on the UMIST face database for different values of  $s$  by varying feature size: (a)  $s=4$ , (b)  $s=6$ , (c)  $s=8$ , (d)  $s=10$



## Experiments on the FERET Face Database

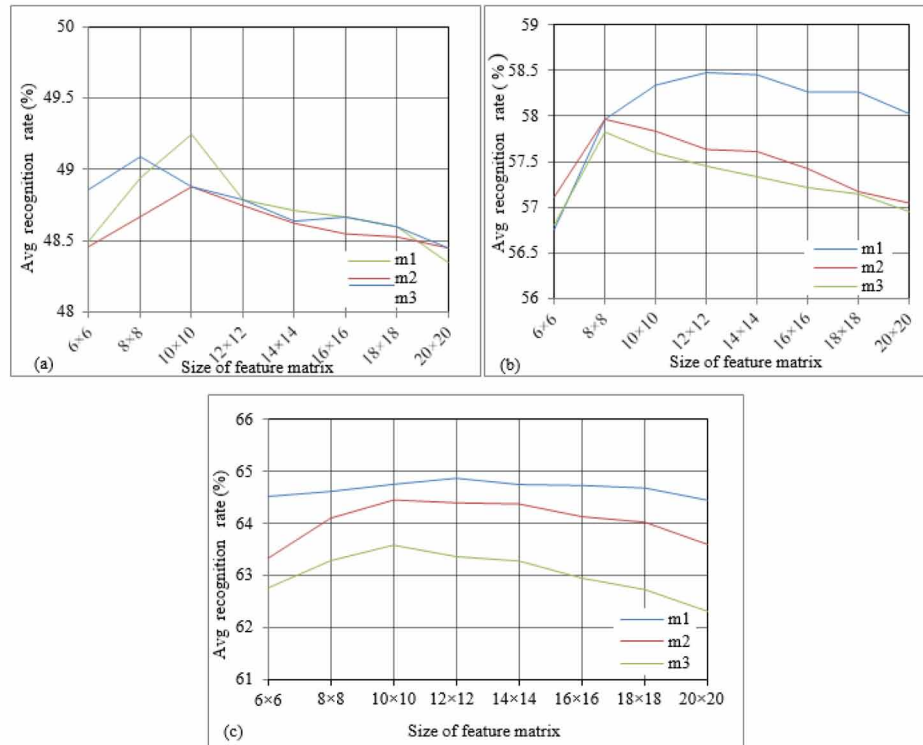
In this Section, the performance of the present method on the FERET face database is discussed. We have briefly described the FERET face database. In this face database, the performance of three proposed fusion methods has been evaluated in this Section. In this experimental strategy, the database is partitioned randomly into training and test sets. The investigation is done by varying the size of the feature matrix from  $6 \times 6$  to  $20 \times 20$  in terms of average recognition rates in 10 experimental runs with different training and test sets. The results in Figure 9 show a comparative study of the m1, m2, and m3 methods over the FERET face database by varying feature size with  $s = 2, 3$  and  $4$  and repeated 10 times with different training and test sets. The analysis once more shows that the m1 method yields better performance and yields average recognition rates of 49.25% ( $10 \times 10$ ), 58.34% ( $10 \times 10$ ) and 64.87% ( $12 \times 12$ ) with 2, 3 and 4 training images/person, respectively. The RBFNN is modeled with 400, 400 and 600 hidden layer nodes for 2, 3, and 4 training samples per person, respectively.

Table 2. Comparison of different methods along with three presented image fusion method in terms of average recognition rates (%) on the UMIST face database by randomly partitioning the database. Figures within the parentheses denote the number of features.

Method	Averagerecognitionrates			
	s= 4	s= 6	s= 8	s= 10
True diagonal imagesuperimposedwithorigi nalimage (m1)	<b>86.56</b> (28×28)	<b>92.37</b> (20×20)	<b>96.7</b> (22×22)	<b>98.02</b> (24×24)
Partialdiagonalimage placedhorizontaland verticalwithoriginal image(m2)	85.13 (18×18)	91.95 (16×16)	96.01 (20×20)	97.36 (16×16)
Partial diagonal imagesuperimposedwithorigi nalimage (m3)	82.99 (28×28)	90.09 (26×26)	94.87 (10×10)	97.35 (10×10)
G-2DFLD	86.22 (14×14)	92.28 (14×14)	95.54 (14×14)	96.92 (14×14)
2DFLD	86.12 (112×14)	92.16 (112×14)	95.25 (112×14)	96.55 (112×18)
2DPCA	85.70 (112×14)	91.91 (112×14)	95.07 (112×14)	96.60 (112×18)
PCA+FLD	76.31 (25)	85.69 (25)	90.93 (25)	93.72 (25)
PCA	80.72 (60)	86.53 (60)	94.01 (60)	95.11 (60)

The comparisons in terms of recognition rates (%) of the other holistic-based methods along with the three proposed fusion methods based on the FERET. Table 3 displays the comparison of performances between the present three fusion technique and some other methods. Table 3 summarize the comparison of performances of these contemporary methods in terms of recognition rates (%). The same radial basis function (RBF) neural network and parameters are used for training, classification and recognition. The empirical results show that the m1 method outperforms the other methods in all experimental runs. This indicates that by using the information both from original and true diagonal images together, it is possible to extract superior is criminative features.

Figure 9. Comparative study in terms of average recognition rates on the FERET face database for different values of  $s$  by varying feature size: (a)  $s=2$ , (b)  $s=3$ , (c)  $s=4$



## CONCLUSION

This Chapter has presented different image fusion techniques for face recognition and presented a detailed performance analysis among them. The objective was to use the all the directional (horizontal, vertical and diagonal) information within the image region for calculation of feature vectors and to see which fusion technique provides superior discriminative features. The fusion is made by three different ways by placing the original captured image and its true/partial diagonal images (i) one-over-other(superimposed), (ii) side-by-side (horizontally) and (ii) up-and-down (vertically). The experimental results and discussions on publicly available AT&T, UMIST and FERET face databases collectively demonstrate that superimposed image between the original and its true diagonal images actually provides superior discriminant features for face recognition as compared to either original or its diagonal image. The methods can be evaluated using deep learning algorithms instead of the RBFNN, which can be a direction of future work. In addition, convolution of feature-level and image-level fusion can be an interesting and challenging work.

Table 3. Comparison of recognition rates with different method on the FERET face database the parentheses denote the number of features

Method	Averagerecognitionrates		
	s= 2	s= 3	s= 4
Truediagonalimagesuperimposedwithoriginal image(m1)	<b>49.25</b> (10×10)	<b>58.34</b> (10×10)	<b>64.87</b> (12×12)
Partialdiagonalimageplacedhorizontaland verticalwithoriginal image (m2)	49.1 (8×8)	58 (12×12)	64.45 (10×10)
Partial diagonal image superimposedwithoriginal image(m3)	48.8 (8×8)	57.83 (10×10)	63.58 (12×12)
G-2DFLD	49.02 (10×10)	57.96 (16×16)	64.24 (12×12)
MD2DPCAwith6direction	48.93 (112×20)	54.83 (112×20)	57.60 (112×20)
MD2DPCAwith4direction	49.36 (112×20)	53.94 (112×20)	57.08 (112×20)
Alternative-2DPCA	48.31 (112×20)	53.21 (112×20)	53.97 (112×20)
(2D)2PCA	47.70 (112×20)	52.36 (112×20)	55.45 (112×20)
2DPCA	47.12 (112×20)	52.66 (112×20)	55.20 (112×20)

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## **KEY TERMS AND DEFINITIONS**

**Face Recognition:** The face of a person can be used to identify or verify the identification of another person through a process known as facial recognition.

**Feature Extraction:** The job of discovering and extracting relevant information or features from a picture is referred to as “feature extraction,” and it is an essential one in the field of image processing.

**Image Fusion:** It is used to integrate information from many photographs of the same scene into a single image that, ideally, retains all of the key aspects from each of the original images. This is accomplished by combining the information from numerous images into a single image.

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## About the Contributors

**Vinod Kumar** received the Bachelor of Science (PCM) from the University of Allahabad, Uttar Pradesh, India in 2008 and the Master of Computer Applications in 2011. He qualified for UGC-NET (Computer Science and Applications) in 2012. He did his Ph.D. from Maulana Azad National Institute of Technology (MANIT), Bhopal (MP) in 2019. He has worked as a Project Fellow on Project “Network Simulation Testbed at MCTE, MHOW (MP)” in collaboration with the Military College of Telecommunication Engineering (MCTE), Mhow (MP), funded by the Army Technology Board. He has over 10 years of experience in research and teaching. Currently, he is working as an Associate Professor in the Computer Science and Engineering Department of Koneru Lakshmaiah Education Foundation (KL Deemed to University), Andhra Pradesh. He is an active researcher in the fields of Big Data Analytics, Web Mining, Machine Learning, Blockchain Technology, and the Internet of Things. He has published 20+ research articles in reputed journals and presented his research work at conferences.

\* \* \*

**A.K. Awasthi**, Professor, Department of Mathematics, School of Chemical Engineering and Physical Sciences, Lovely Professional University, Punjab, India. M.Sc, LL.B, Ph.D. (Mathematics), D.Sc (contd.) Harcourt Butler Technological Institute, Kanpur. Prof. A.K. AWASTHI has earned his Ph.D. from Harcourt Butler Technological Institute, Kanpur, India. He has total teaching, research & administrative experience of more than 22 years with many reputed universities. He worked at Manav Rachna University as a HOD in the Department of Mathematics from Aug. 2012 to 2019. During tenure established the faculty of Applied Sciences with three Mathematical labs for each subject of mathematics namely Techno Math lab for Engineers, Computational Math lab for M.Sc, B.Sc Programme of Physics, Chemistry, Maths & Eco Math lab for BBA, and MBA scholars. Designed Special Curriculum for M.Sc, and B.Sc programs with Lab Components especially in each Math subject. Prof. Awasthi is associated as an editor of two forthcoming books with CRC Press and Scrivener Publishing (Wiley) respectively. He is a special issues editor in the journal EAI Endorsed on Transactions on Pervasive Health and Technology (Scopus Indexed). He is associated with the International Journal of Communication Systems (SCIE) (WILEY), and International Journal of Information Security and Privacy (IJISP) (Scopus, ESCI), and IGI Global as an active reviewer. He has guided eight Ph.D. research scholars and supervised seven in the fields of Applied Mathematics and Computing. He is a lifetime member of the Indian Engineering Teachers Association, India, and other renowned technical societies. He is holding the post of Joint Secretary, Faridabad Chapter of INDO-UK Confederation of Science Technology and Research, London. He is a certified Microsoft Technology Associate for Introduction to Programming using Python. Prof.

Awasthi has got more than 100 publications in refereed journals and 78 publications in National and International conferences. He has also written and reviewed many books like Topology, Real Analysis, Integral Transform, and Complex Analysis for Master & Research courses.

**Arpit Jain** is Professor at Koneru Lakshmaiah University Education Foundation, Vijayawada, A.P., India. He has more than 17 years of Academic and Research. In his 17+ years of Experience, he has been able to bring out best from individuals and create a healthy work environment, with the changing work demand. He has been able to write about more than 40+ research papers including the SCI Journal, Scopus Journal, UGC Care List, Web of Science on area ranging from Digital Image Processing to Network on Chip Implementation with a backdrop of improving the Chip performance and utility. Dr. Jain is the member of various Professional Societies like IEEE, Computer Society of India, ISTE, ACM and more. He has also filed the 25+ patents on National and International level. His Research areas are Digital Image Processing, Machine Learning, Convolutional Neural Network and Chip Implementation.

**Nimish Kumar** is a highly accomplished computer scientist and engineer with over 24 years of experience in industry and academia. He holds a BE, MTech and a PhD degree in Computer Science and Engineering, all from reputed universities. Dr. Kumar's area of specialization is Artificial Intelligence and Software Reliability, and his areas of interest include Neural Networks, Internet of Things (IoT), Computer Vision, and Data Structures. He has published numerous research papers in top international and national journals and conferences, which have been widely recognized in the field. He currently serves as the Head of Department for Computer Science and Engineering (CSE), Information Technology (IT), Artificial Intelligence (AI), and Data Science (DS) at BK Birla Institute of Engineering and Technology in Pilani (Raj). Dr. Kumar is also an accomplished author and has written three books on the subject of Artificial Intelligence and IoT. He is highly respected by his peers and students, and his passion for research and teaching continues to inspire the next generation of computer scientists and engineers.

**Manish Maheshwari** is currently working as professor at Department of Computer Science and Applications, Makhanlal Chaturvedi National University of Journalism and Communication, Bhopal. He has more than 25 Years of teaching experience at undergraduate and postgraduate level. Dr Maheshwari holds Doctorate, Masters and Bachelor's degree in Computer Science and Engineering. His areas of interest includes Data Mining, Image retrieval, Neural Network and Machine Intelligence. He has made several publications in conferences, national and international journals.

**Sasikala Ponnusamy** is HoD of New Media Technology, Makhanlal Chaturvedi National University of Journalism and Communication, Bhopal, India.

**Himanshu Prajapati** is pursuing his B.Tech (CSE) in United Institute of Technology (UIT), Prayagraj, India.

**Yogesh Kumar Sharma** is presently working as a Professor in the department of Computer Science and Engineering at Koneru Lakshmaiah Education Foundation (K L Deemed to be University), Vaddeswaram, Guntur District, AP. He has 16 years teaching and 08 years' research experience. He completed his Ph.D. in Computer Science, from "Shri J.J.T. University", Jhunjhunu, Rajasthan in the year 2014. In his research career he published more than 173 Papers in National as well as International

### **About the Contributors**

reputed journals, He published 04 patents & 09 Books in National & International Publication. Under his guidance 14 research scholars awarded Ph.D. Degree.

**Ganga Devi** received her Bachelor's degree (B.Sc.) from S.V. University, Tirupati; her Master's degree in Computer Applications (M.C.A.) from Sri Padmavathi Mahila Visva Vidyalayam (Women's University), Tirupati; and her Ph.D. in Computer Science from Sri Padmavathi Mahila Visva Vidyalayam (Women's University), Tirupati. She has presented and published various papers in international and national journals and conferences. She has 27 years of teaching and 13 years of research experience. Her research interests are data mining, soft computing, data science, databases, fuzzy logic, and deep learning.

**Himanshu Verma** received his master's degree in Embedded Systems from Jaipur national university, Jaipur in 2010. He has more than 16 years of teaching and industry experience. He worked as a developer in the Japanese tech industry in Tokyo. Currently, he is working as assistant professor at B K Birla Institute of Engineering and Technology, Pilani. He has conducted several training programs for engineering faculty sponsored by MHRD, ISTE, RTU Kota and NITTTR Chandigarh. He has also conducted sponsored workshops and faculty development programs on topics Embedded World, Cyber Crime and Forensic Tools, Aakash Android Application Programming, VLSI System Design to name a few. He is nominated as a chairman of IEI (PLC). He is a member of various professional bodies such as Institution of Engineers (India), International Association of Engineers Hong Kong and International Academy for Science & Technology Education and Research. His research interests include Machine Learning, Image Processing, Pattern Recognition and Artificial Intelligence.

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