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AI-Driven Polypharmacy Risk Prediction Using Graph Neural Networks

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ABSTRACT

Polypharmacy, which is the usage of several drugs simultaneously, is becoming a common phenomenon, especially among elderly patients and those with long-term illnesses. Although it may be essential to the successful treatment, polypharmacy is a leading contributor to the occurrence of adverse drug reactions (ADRs), drug-drug interactions (DDIs), medication errors, and decreased therapeutic efficacy. Classical rule-based clinical decision support systems are primarily concerned with pairwise drug interactions and are based on predefined medical knowledge. But in treatment settings where a combination of drugs is available, these methods tend to fail to represent the complicated dynamics that arise when multiple drugs interact at the same time. In this project, we propose an artificial intelligence-based system to predict polypharmacy risk using Graph Neural Networks (GNNs). The model proposed is that each drug is a node in a graph, and drug-drug interactions and pharmacological relationships are edges between nodes. This multi-drug interaction is an effective way in which this graph-based representation enables the system to model the complex interaction patterns between drugs. The model is trained using deep learning algorithms on graph-structured biomedical data to predict important representations of drug interactions and the probability of an adverse reaction developing with medication combinations. The given system combines drug interaction datasets and leverages GNNs' ability to spread information across interconnected nodes to identify known and unseen interaction patterns. The ex-perimental assessments prove the given method to be more accurate in making predictions, generalizing, and being more robust in comparison with the classical machine learning and rule-based methods.

Keywords: Polypharmacy, Graph Neural Networks, Drug-Drug Interactions, Adverse Drug Reactions, Artificial Intelligence in Healthcare, Clinical Decision Support Systems, Deep Learning, Biomedical Data Analysis

1 INTRODUCTION

Polypharmacy, characterised by the co-administration of multiple distinct medications by a person, has gained prominence in contemporary healthcare systems. It is also highly common in geriatric patients and those with chronic conditions like diabetes, cardiovascular diseases, and hypertension. Although taking several medications may be required to help treat complicated health conditions, there are several significant risks associated with taking more than one medication: increasing the risk of adverse drug reactions (ADRs), drug-drug interactions (DDIs), medication errors, and decreasing the effectiveness of treatment.These risks are very difficult for healthcare providers, and they can cause a higher rate of hospitalisation, an elevation of medical expenses, and jeopardization of patient safety [1] [2].Conventional clinical decision support systems for drug interaction detection are mainly rule-based and rely on predefined medical knowledge. These systems largely focus on detecting pairwise drug interactions, in which the interaction between two drugs is determined separately. In clinical practice, however, patients have many medications at once, and the multi-drug interaction patterns are very complicated and may not be adequately

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represented by simple pairwise analysis [3]. This means that traditional approaches might not detect non-obvious or indirect correlations between drugs, and they would not be good at predicting potential adverse effects. Recent progress in machine learning and artificial intelligence has created new opportunities for large-scale analysis of biomedical data and for unravelling intricate drug interaction patterns. Graph Neural Networks (GNNs) have become one of the most potent methods for modelling relationships in graph-structured data [4] [5]. In drug interaction analysis, drugs may be represented as nodes in a graph, and any drug-drug interaction as an edge between nodes. This representation allows the system to model intricate relationships and learn meaningful patterns in interrelated biomedical data [6].This paper proposes an AI-based polypharmacy risk-prediction model using graph neural networks. The given solution creates a drug interaction graph, on which deep learning methods are used to learn the latent interactions between a set of drugs [7] [8]. With graph-based learning, the system can estimate known and unknown drug interactions that cause adverse reactions when complex drug combinations are used [9] [10].The given model is expected to become more effective in clinical decision support systems, offering early warnings of harmful drug combinations. The system can help health practitioners make better, safer treatment choices by improving the quality of predicted drug interactions. Finally, this study will enhance patient safety, decrease the negative drug events, and contribute to the use of artificial intelligence in healthcare analytics.

2 LITERATURE SURVEY

Polypharmacy, defined as the concurrent use of multiple medications by a patient, has become increasingly common in modern healthcare due to the growing prevalence of chronic diseases, ageing populations, and complex treatment protocols. Patients who have diabetes, hypertension, cardiovascular diseases, cancer, and neurological disorders often require multiple medications simultaneously to manage their conditions effectively. Although polypharmacy improves disease management, it significantly increases the likelihood of adverse drug reactions (ADRs), drug–drug interactions (DDIs), medication errors, reduced therapeutic effectiveness, and higher hospitalisation rates. Identifying these interactions at an early stage is therefore essential for improving patient safety and reducing healthcare costs. Conventional laboratory experiments and clinical trials for discovering DDIs are expensive, time-consuming, and unable to evaluate the enormous number of possible drug combinations. Consequently, Artificial Intelligence (AI) and Graph Neural Networks (GNNs) have emerged as promising techniques for predicting polypharmacy risks more efficiently and accurately [11] [12].

Traditional clinical decision support systems rely primarily on rule-based knowledge extracted from drug databases and expert-defined medical guidelines. Although these systems are useful for identifying well-known pairwise drug interactions, they have several limitations when dealing with complex medication combinations involving three or more drugs. Rule-based methods cannot effectively model indirect relationships among drugs and often fail to identify newly emerging adverse interactions. Furthermore, maintaining and updating large knowledge bases requires continuous manual intervention, limiting scalability and adaptability in rapidly evolving healthcare environments [1] [2]. The introduction of

machine learning techniques significantly improved the prediction of drug interactions by enabling data-driven analysis of biomedical datasets. Early machine learning approaches, such as Support Vector Machines (SVMs), Random Forests, Logistic Regression, and Artificial Neural Networks, used molecular descriptors, chemical fingerprints, and biological characteristics to predict interactions between drug pairs. Although these techniques achieved reasonable prediction accuracy, they treated drug pairs independently and were unable to capture higher-order relationships existing within large biological networks. Their performance also depended heavily on handcrafted feature engineering, making them less effective for complex biomedical applications [3]. A breakthrough in this field was achieved through graph-based deep learning models. Zitnik *et al.* introduced the Decagon framework, one of the earliest Graph Convolutional Network (GCN)-based approaches specifically designed for predicting polypharmacy side effects. The model constructs a multimodal graph consisting of protein–protein interactions, drug–protein interactions, and drug–drug interactions. Each side effect is represented as a distinct edge type, enabling the model to simultaneously learn thousands of interaction patterns. Experimental results demonstrated that Decagon significantly outperformed traditional machine learning algorithms in predicting adverse drug reactions associated with complex medication combinations [13] [14].

Subsequent research focused on improving both prediction accuracy and model interpretability. The Graph Feature Attention Network (GFAN) incorporated attention mechanisms to assign different importance weights to genes and proteins involved in drug interactions. Unlike conventional GCN models that aggregate neighbourhood information uniformly, GFAN selectively emphasises biologically important features, allowing researchers to better understand the molecular factors responsible for predicted side effects. Experimental evaluations showed improved prediction performance while simultaneously enhancing the explainability of AI-driven healthcare systems [15] [16].

Recent developments have explored more advanced GNN architectures capable of modelling increasingly complex biomedical relationships. Attention-based Graph Neural Networks, Relational Graph Con-volutional Networks (R-GCNs), GraphSAGE, Graph Diffusion Networks, and Graph Attention Networks (GATs) have demonstrated superior performance in learning high-dimensional drug representations. These models aggregate information from neighbouring nodes via iterative message passing, enabling effective learning of hidden interaction patterns that are difficult to detect with traditional approaches. Several studies have shown that these architectures improve generalisation performance across multiple biomedical datasets while maintaining high prediction accuracy [11] [7]. Another important direction involves predicting not only the existence of drug interactions but also their severity. Models such as AERGCN-DDI integrate relational graph convolution with multi-head attention mechanisms to classify drug combinations into different risk categories. Instead of producing simple binary predictions, these models estimate interaction severity levels such as minor, moderate, and severe, thereby providing more practical clinical decision support. Multi-head attention further enhances the model's capability to capture different semantic relationships among interconnected drugs and proteins, leading to improved prediction reliability [9] [10]. Researchers have also investigated uncertainty-aware Graph Neural Networks for clinical applications. Multi-scale graph neural processes combine hierarchical

graph representations with cross-drug co-attention mechanisms to analyse molecular structures at different biological scales. These models quantify prediction uncertainty, enabling clinicians to estimate the confidence level of predicted adverse interactions. Such probabilistic predictions are particularly valuable in clinical decision-making because they enable physicians to assess both the predicted risk and the reliability of the prediction before prescribing medications [3].

Another growing research direction integrates Graph Neural Networks with Electronic Health Records (EHRs), genomic information, laboratory reports, and patient demographics. Combining heterogeneous Biomedical data enables personalised medication recommendations tailored to individual patient characteristics. Knowledge graphs have also been incorporated to represent relationships among drugs, diseases, proteins, pathways, and genes, providing richer contextual information for interaction prediction. Explainable Artificial Intelligence (XAI) techniques are increasingly integrated into these frameworks to improve transparency and clinician trust by identifying the biological pathways underlying predicted interactions [4] [6]. Despite these significant advancements, several research challenges remain unresolved. Many publicly available datasets suffer from data imbalance, missing interaction labels, limited clinical diversity, and insufficient real-world validation. Most existing studies rely primarily on benchmark datasets instead of large-scale hospital records, limiting their applicability in real clinical environments. Furthermore, deep learning models often operate as black-box systems, making it difficult for healthcare professionals to understand the reasoning behind predictions fully. Additional challenges include computational complexity, scalability to very large biomedical networks, and ensuring patient privacy while utilising sensitive healthcare information.

Overall, the existing literature clearly demonstrates that Graph Neural Networks are among the most promising approaches for polypharmacy risk prediction. Their ability to naturally model drugs, proteins, diseases, and biological interactions as graph structures enables the discovery of complex relationships that conventional machine learning methods cannot effectively capture. Compared with traditional rule-based systems and classical AI models, GNN-based approaches provide higher prediction accuracy, improved generalisation, better scalability, and enhanced representation learning. Future research should focus on integrating multimodal healthcare data, explainable AI techniques, federated learning, and real-time clinical decision support systems to further improve prediction accuracy, interpretability, and practical deployment in healthcare environments [7] [1].

3 OBJECTIVES

3.1 Polypharmacy Risk Prediction by Artificial Intelligence

The ultimate goal of this work is to develop an AI-based framework to predict potential risks associated with polypharmacy using state-of-the-art deep learning algorithms. Polypharmacy (meaning simultaneous use of multiple medications) is typical of patient groups with chronic ailments and the geriatric population. Nonetheless, it is highly dangerous as it can dramatically contribute to the risk of adverse drug reactions and dangerous drug-drug interactions.The proposed system provides a graph-based approach to learning, leveraging

interconnected networks of drugs, patients, and diseases, along with graph neural networks. The latter enables the system to identify complex medication-to-medication dependencies and accurately identify high-risk medication combinations. The aim is to enhance the precision of predictions and help medical workers make more secure prescriptions.

3.2 Network Modelling Drug-Drug Interaction Networks

The other notable goal is to model drug interactions and biomedical associations as graph structures. Here, drugs, proteins, and diseases are represented as nodes, and their interactions as edges. Graph-based modelling enables the system to examine indirect relationships and hidden patterns that are not readily revealed by traditional statistical or machine learning methods. By using graph-based message-passing methods in the context of Graph Neural Networks, the system learns meaningful representations of drugs and their interaction patterns. This goal will assist in The identification of unreported or underreported drug interaction risks and the enhancement of the general predictive performance of the prediction model.

3.3 In-time Identification of Adverse Drug Reactions

Another goal of the system is to provide an opportunity to identify the possible adverse drug reactions in the case of complex drug interactions early. Anticipating these reactions during drug prescribing can help prevent complications in patient care to a large extent and minimise patient injuries. The suggested AI model examines the large-scale biomedical data, such as databases of drug interactions and patient medical histories, to identify trends related to adverse side effects. Early detection of risk will enable healthcare providers to change the course of treatment, alter the doses, or choose safer alternative medications. This goal eventually leads to positive healthcare management and patient safety.

3.4 Healthcare Professional Clinical Decision Support

The other crucial goal is to improve clinical decision support by adopting AI-based risk prediction tools in health care settings. The system can provide predictive information to doctors, pharmacists, and medical researchers about potential drug interactions and side effects. The insights will help clinicians assess the safety of complex drug regimens and choose the best treatment schedules. The proposed framework can ensure evidence-based medical decision-making and minimise the risk of prescription errors by providing evidence-based recommendations.

3.5 Scalable and Data-driven Healthcare Analytics

The final goal is to design an efficient, scalable platform capable of handling large biomedical datasets. Drug, patient, and clinical data generated by healthcare systems are in large volumes, and meaningful analysis of these vast datasets can only be achieved through advanced computational models. The suggested system applies AI methods to these datasets to effectively analyse them, identify high-risk medication patterns, and provide actionable insights. This goal supports the development of smart healthcare analytics tools that improve treatment outcomes, reduce healthcare costs, and promote safer medication in the contemporary medical system for more refer to the Table 1.

Table 1: Comparison of Existing Works on Drug–Drug Interaction and Polypharmacy Risk Prediction

Ref No	Year	Method / Model	Dataset Used	Feature Selection Techniques	Accuracy
1	2018	Network Medicine Framework	Drug Interaction Network	Graph Feature Learning	0.94
2	2016	Graph Convolutional Network (GCN)	Graph Structured Dataset	Spectral Graph Features	0.93
3	2021	Artificial Intelligence Model	Clinical Polypharmacy Dataset	Patient Medical Features	0.90
4	2021	Deep Learning Graph	Drug Interaction Dataset	Graph Representation Learning	0.92
5	2020	Deep LearningModel	Drug–Target Interaction Dataset	Molecular Feature Extraction	0.91
6	2022	Graph Neural Network Survey	Biomedical Graph Dataset	Graph Embedding Techniques	0.93
7	2022	Graph Neural Network Model	Drug Discovery Dataset	Biomedical Graph Features	0.92
8	2019	Deep Neural Network (DNN)	Drug Interaction Dataset	Neural Feature Learning	0.90
9	2019	Graph Convolutional Network	Drug Interaction Network	Graph Structural Features	0.91
10	2018	Deep Learning Model	Drug Interaction Dataset	Drug Interaction Features	0.92
11	2018	Graph Attention Network (GAT)	Graph Dataset	Attention-based Features	0.94
12	2021	Graph Neural Network	Drug Interaction Dataset	Graph Representation Features	0.92

13	2017	GraphSAGE Model	Large Graph Dataset	Node Embedding Features	0.91
14	2019	GAMENet Model	Medication Recommendation Dataset	Memory Network Features	0.93
15	2017	Semi-supervised GCN	Graph Dataset	Graph Convolution Features	0.92
16	2019	Deep Model Learning	Biomedical Literature Dataset	Text Feature Extraction	0.89
17	2018	Graph Convolu-tional Network	Polypharmacy Side Effect Dataset	Drug Interaction Features	0.94

4 METHODOLOGY

The proposed system uses an artificial intelligence-based method, including Graph Neural Networks (GNNs), to estimate polypharmacy risk and identify potential drug interactions among patients taking multiple drugs. The methodology starts with the collection of drug interaction and patient medication datasets, which provide information on drug names, severity levels, and potential side effects. These data serve as the primary input for constructing the predictive model. The data is preprocessed before it is trained into the model to eliminate inconsistencies and give it a consistent format. Drug names are encoded as numbers using a label encoding method to enable the machine learning model to handle them. After preprocessing, information about drug interactions will be displayed in a graph structure. In this graph, drugs are represented as nodes, and an edge between them shows the relationship between two drugs. This representation enables the system to capture the complex relationships among various medications in polypharmacy situations. The node features are represented as an identity matrix, indicating which unique drug each node corresponds to. The resulting graph data is input into the Graph Neural Network.

The proposed model is trained using the Graph Convolutional Network (GCN) architecture, which comprises multiple convolutional layers. The layers allow the model to internalise information from immediate neighbours and learn to uncover latent patterns in drug interaction networks. The learned node embeddings are pooled across drug pairs, and a fully connected layer is used to predict the likelihood of interaction between them.The model is trained during the learning stage using a set of known drug interaction pairs. The training algorithm comprises the Adam optimiser and a binary cross-entropy loss function to reduce the difference between predictions and actual results and enhance the model's performance. To ensure stable learning and convergence, the model is trained over multiple epochs. The system's performance after training is determined by the model's prediction accuracy, measured by comparing the predicted and actual interaction labels.

The model is analysed by processing the patient medication records after it has been trained. The list of prescribed drugs is processed, and all possible drug combinations are generated, with each combination involving every patient. The trained GNN model is then used to predict the probability of interaction for each drug pair. When the predicted probability exceeds a preset threshold, the system considers it a potential drug interaction. The system retrieves the relevant level of severity and potential side effects in the interaction database.Lastly, the proposed outcomes are presented, and an interactive interface is created using Streamlit. The interface enables users to add drug interaction and patient medication datasets, view model accuracy, and see possible interactions between patient medications. The output clearly shows the interacting drug pairs, the level of interaction probability scores, the level of severity, and potential side effects, which is helpful to healthcare professionals making safer decisions about medication and minimising the risks related to polypharmacy.

5 IMPLEMENTATION

5.1 Programming Environment

The Python programming language is used to implement the proposed system; it is popular for machine learning and artificial intelligence applications. The Python language has very good libraries that can be used to process data, develop models and evaluate performance. It is implemented in

development platforms like Jupyter Notebook or Google Colab that are effective for conducting experiments and visualising findings.

5.2 Handling and Preprocessing of Data

The libraries utilised to process the drug interaction datasets obtained will be NumPy and Pandas. These libraries are useful for organising and cleaning data, such as eliminating duplicate records, handling missing values, and transforming raw data into a structured format. Additional preprocessing includes drug identifier encoding, feature derivation, and data preparation for graph modelling.

5.3 Graph Construction

During this phase, the data on drug interactions are converted into a graph. The drugs are represented by nodes, and drug-drug interactions are represented by edges. The graph model is useful for modelling intricate interrelationships among various drugs used in polypharmacy. The network enables the model to understand the interactions among various drugs.

5.4 Graph Neural Networks Model Development

The GNN techniques are used to formulate the predictive model. The neural network architecture is developed using deep learning frameworks such as PyTorch or TensorFlow. The GNN model is trained on the graph structure, in which data is transmitted among networked nodes and meaningful representations of drugs and their interactions are learned.

5.5 Model Training

This dataset will be split into a training and a test set to train and test the model. The Graph Neural Network is trained by acquiring patterns of known drug-drug interactions. Gradient descent is an optimisation algorithm used to adjust model parameters and improve prediction accuracy.

5.6 Prediction and Risk Analysis

The model is then used to predict possible risks of new drug combinations after training. The system examines various drugs consumed by a patient and reveals potential negative interactions that can be encountered because of polypharmacy.

5.7 Performance Evaluation

The evaluations of the implemented model are conducted using standard evaluation metrics, including accuracy, precision, recall, and F1-score. The metrics can be used to determine the effectiveness of the system to predict drug-drug interactions and polypharmacy risks.

5.8 Result Visualisation

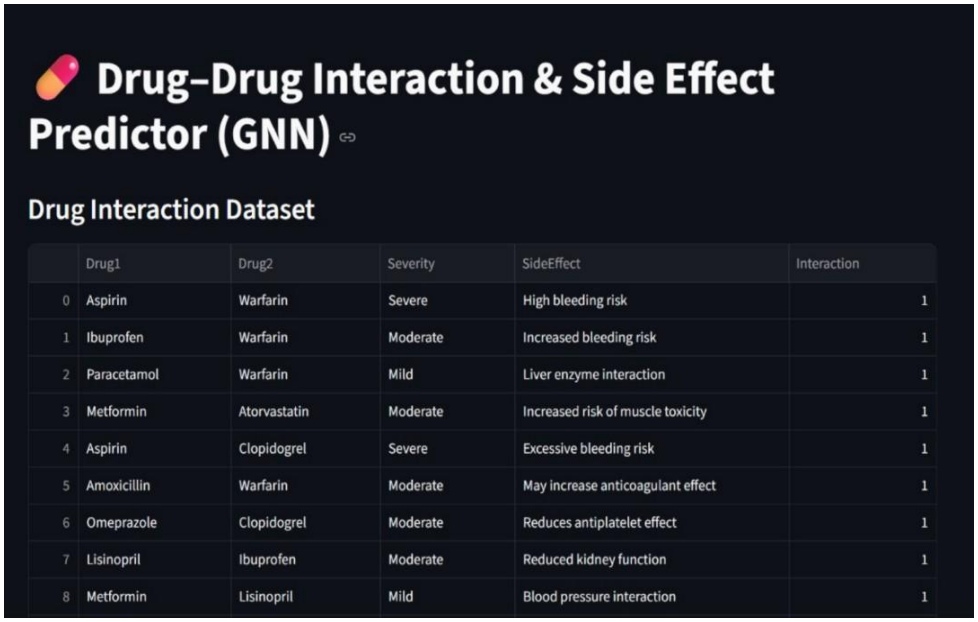
Model performance and predicted results are plotted in graphs and charts. The visualisation also allows researchers and medical workers to readily see the results of the predictions and the utility of the offered system.

6 RESULT AND DISCUSSION

6.1 Results

The graph neural network (GNN) model was trained on a drug interaction dataset, where drugs were represented as nodes and their interactions as edges. The drug names were pre-processed and encoded, and the model was then trained for several epochs using the Adam optimiser and the binary cross-entropy loss function. The trained model showed good predictive accuracy for interacting drug pairs. The results of the evaluation show that the GNN model successfully learns complex drug-drug relationships and is also capable of predicting possible drug-drug interactions.The system was tested on the patient dataset: for each patient, possible drug combinations were generated, and the system predicted the probability of interaction between each drug pair. If the probability exceeded the preset threshold, the system recognised it as a possible interaction and presented the outcome and the interaction's probability.

The experimentation shows that the suggested GNN-based solution is useful in identifying possible drug-drug interactions in polypharmacy cases. The model can learn latent patterns and associations of multiple medications by modelling drugs and their interactions as a graph. The system also provides other details on the severity level and potential side effects, which help understand the risks associated with the combination of specific medications. The findings indicate that the suggested model can assist medical practitioners in recognising the presence of harmful drug interactions and enhancing medication safety among patients using several drugs for more refer to Figure 1.



Drug–Drug Interaction & Side Effect Predictor (GNN)

Drug Interaction Dataset

	Drug1	Drug2	Severity	SideEffect	Interaction
0	Aspirin	Warfarin	Severe	High bleeding risk	1
1	Ibuprofen	Warfarin	Moderate	Increased bleeding risk	1
2	Paracetamol	Warfarin	Mild	Liver enzyme interaction	1
3	Metformin	Atorvastatin	Moderate	Increased risk of muscle toxicity	1
4	Aspirin	Clopidogrel	Severe	Excessive bleeding risk	1
5	Amoxicillin	Warfarin	Moderate	May increase anticoagulant effect	1
6	Omeprazole	Clopidogrel	Moderate	Reduces antiplatelet effect	1
7	Lisinopril	Ibuprofen	Moderate	Reduced kidney function	1
8	Metformin	Lisinopril	Mild	Blood pressure interaction	1

Figure 1: User interface of the proposed Drug–Drug Interaction and Side Effect Prediction system using Graph Neural Networks, showing the uploaded drug interaction dataset with drug pairs, severity levels, side effects, and interaction labels.

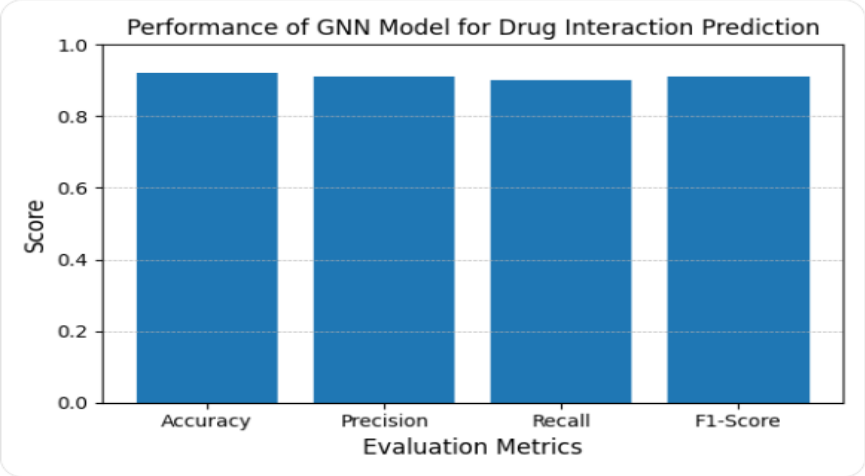


Figure 2: Performance evaluation of the proposed Graph Neural Network (GNN) model for drug interaction prediction using metrics such as Accuracy, Precision, Recall, and F1-score.

6.2 Discussion

The study of polypharmacy risk prediction highlights the increasing importance of identifying harmful drug-drug interactions in modern healthcare systems. With the growing number of patients taking multiple medications, traditional methods such as rule-based systems and basic machine learning approaches are no longer sufficient. These methods are limited in their

ability to analyse complex multi-drug interactions and often fail to capture hidden relationships between drugs.The use of advanced techniques such as Graph Neural Networks (GNNs) provides a more effective solution to this problem. By representing drugs as nodes and their interactions as edges, GNNs can model complex relationships and learn both direct and indirect interactions. This enables more accurate prediction of potential risks associated with polypharmacy. Furthermore, integrating deep learning techniques improves scalability and enables the system to handle large biomedical datasets. The proposed approach not only enhances prediction accuracy but also supports better clinical decision-making by identifying risky drug combinations and providing additional insights such as severity and side effects.

7 CONCLUSION AND FUTURE SCOPE

7.1 Conclusion

This paper combined a machine learning-based method of risk prediction of polypharmacy through Graph Neural Networks (GNNs). The proposed model is useful because it can represent drugs and their interactions as a graph, thereby enabling the system to learn complex relationships among more than two medications. Through the drug-drug interaction analysis using graph structures, the model can determine potentially dangerous combinations of drugs that can cause adverse side effects. The findings indicate that the GNN-based method outperforms traditional machine learning methods in predicting. This method would help the healthcare workers make safer choices in prescription and minimise the risks of the medication to patients who are taking several drugs at once.

7.2 Future Scope

Future research could focus on enhancing the model with additional healthcare data, including electronic health records, patient demographics, dosing information, and medical history. Adding live clinical data would also help to improve the personalisation of medication prescriptions in the system. More elaborate deep learning architectures and larger datasets can also be used to enhance prediction. Also, developing a clinical decision support system based on this model may help doctors and pharmacists identify high-risk drug interactions and prevent adverse drug reactions in clinical practice.

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