GNN – Enhanced Drug Interaction Detection and Adverse Reaction Analysis with Sentiment Insights

Dr.SV.SHRI BHARATHI
Department of Data Science and Business Systems
SRM Institute of Science and Technology
Kattankulathur, Tamil nadu
shribharathi01@gmail.com

ABISEK KAMTHAN R S
Department of Data Science and Business Systems
SRM Institute of Science and Technology
Kattankulathur, Tamil nadu
abisek971@gmail.com

VENKATADURGA PRANESH B
Department of Data Science and Business Systems
SRM Institute of Science and Technology
Kattankulathur, Tamil nadu
pranesh.b06@gmail.com

HARITH BALA
Department of Data Science and Business Systems
SRM Institute of Science and Technology
Kattankulathur, Tamil nadu
harithbala62850@gmail.com

GAURANG SRIVASTAVA
Department of Data Science and Business Systems
SRM Institute of Science and Technology
Kattankulathur, Tamil nadu
gaurangsrivastava16@gmail.com

Dr. G. Divya
Department of Data Science and Business Systems
SRM Institute of Science and Technology
Kattankulathur, Tamil nadu
mailtodivya16@gmail.com

***Abstract*— This study presents a novel approach for identifying Drug-Drug Interactions (DDIs) and forecasting Adverse Drug Reactions (ADRs) by integrating Graph Neural Networks (GNNs) with Sentiment Analysis. Unlike conventional models that primarily focus on molecular interactions, our method integrates molecular data with real-world patient-reported outcomes to provide a more comprehensive drug safety assessment. By leveraging GNNs to model complex drug relationships and analyzing sentiment from the FDA's Adverse Drug Reaction database, our framework enhances predictive accuracy. Experimental results demonstrate that our model outperforms existing approaches, achieving an AUC of 0.981, an AUPR of 0.983, and an accuracy of 0.997. This integration not only improves the detection of DDIs but also quantifies their severity more effectively, offering a robust and clinically relevant tool for improved drug safety and decision-making.**

Keywords—Graph Neural Networks (GNN), Drug-Drug Interactions (DD), Adverse Drug Reactions (ADR), Sentiment Analysis

I. Introduction

Medications are essential in managing medical conditions, but they often carry the risk of Adverse Drug Reactions (ADRs), that are unintended and potentially harmful effects. According to the World Health Organization (WHO), ADRs account for approximately 5% of all hospital admissions and are responsible for nearly 197,000 deaths annually in Europe alone. Similarly, Drug-Drug Interactions (DDIs) contribute significantly to adverse outcomes, with studies estimating that around 22% of patients on multiple medications experience clinically relevant DDIs, leading to increased hospitalization rates and healthcare costs.

A significant contributor to ADRs is Drug-Drug Interactions (DDIs), in which the concurrent administration of multiple drugs leads to either enhanced or diminished effects, increasing the risk of complications [8]. The growing use of pharmaceuticals, particularly in complex medical regimens, has intensified the need for improved detection and prediction of harmful drug interactions [9].

Traditional models for DDI detection often focus solely on molecular interactions between drugs, neglecting the valuable real-world insights provided by patient experiences. Many existing approaches, such as knowledge graph-based models and machine learning classifiers, rely primarily on curated databases like DrugBank, which, while valuable, do not account for patient-reported experiences and real-world adverse effects.

This limitation has motivated the exploration of new approaches that combine molecular data with patient feedback to create a more comprehensive understanding of drug safety. In this context, advanced techniques such as Graph Neural Networks (GNNs) and Sentiment Analysis (SA) offer promising avenues for improving DDI prediction [2][3]. GNNs are particularly effective in capturing complex relationships between drugs, while sentiment analysis enables the extraction of meaningful insights from patient-reported outcomes. By integrating these two methodologies, our framework provides a comprehensive and clinically relevant tool for predicting drug interactions and assessing the severity of their adverse effects.

This study aims to enhance drug safety by integrating GNNs to model complex relationships between drugs and Sentiment Analysis to capture patient-reported outcomes. By leveraging both molecular data and real-world patient feedback, we propose a more robust framework for predicting drug interactions and assessing the severity of their adverse effects. Our approach addresses the limitations of existing models by providing a more holistic and clinically relevant tool for drug safety assessments.

II. *Literature Survey*

This literature survey aims to explore the advancements in Drug-Drug Interaction (DDI) prediction, Drug-Target Interaction (DTI) models, and drug recommendation systems, focusing on the integration of machine learning methods, graph neural networks (GNNs), and sentiment analysis.

A. GNN–Based Drug Interaction Prediction

Recent studies have made significant strides in using GNNs to improve predictions for Drug-Target Interactions (DTIs) and DDIs. Uxia Veleiro et al. (2024) proposed GENNIUS, an ultrafast drug-target interaction inference method based on GNNs, improving DTI predictions by incorporating graph representations of drug interactions [1].

Yue Yu et al. (2021) presented SumGNN, a model for multi-typed DDI prediction, which efficiently summarizes knowledge graphs to reduce computational load and improve performance in predicting DDIs [2]. These GNN-based models demonstrate a promising way to improve DTI/DDI prediction by capturing complex relationships between drugs and their interactions. However, their use comes at a cost, particularly in terms of computational resources. While GENNIUS offers ultrafast predictions, it is often too computationally expensive for smaller institutions, making it less accessible [1].

In contrast, SumGNN is designed to be more efficient and suitable for resource-limited environments, although it still faces challenges in handling the quality of data [2].

Additionally, Tanna et al. (2022) explored the application of GNNs in predicting drug interactions within clinical and real-world datasets, underscoring the growing need for large-scale data integration [6].

B. Sentiment Analysis in Drug Safety

Sentiment analysis has emerged as a valuable tool in drug recommendation systems, particularly in leveraging patient feedback from drug reviews. B. Lokeswara Nayak et al. (2022) explored the use of sentiment analysis for drug recommendations based on the sentiments expressed in patient reviews, providing insights into the efficacy and side effects of drugs as perceived by users [3]. Priyanka V. G. (2023) and Satvik Garg (2021) similarly employed sentiment analysis to develop personalized drug recommendation systems, considering user sentiment to improve the precision of recommendations [4][5].

These approaches enhance the ability of drug recommendation systems to reflect real-world patient experiences, which traditional molecular-based systems do not incorporate. Lavanya and Praveen (2022) explored improving recommendation systems through sentiment analysis by considering user preferences and medical feedback, adding an additional layer of personalization to drug suggestions [7].

C. Challenges in Drug Recommender Systems

Despite advances, drug recommendation systems face several challenges, including data management issues and limitations in processing user reviews effectively. Yash Ritesh Tanna et al. (2022) discussed the drawbacks of existing systems, particularly the challenge of dealing with unstructured patient feedback and how this can lead to inefficiencies in predicting the best medications for patients [6]. Similarly, GV Lavanya (2022) highlighted the difficulty in managing large-scale data, particularly in ensuring that drug recommendations are not only personalized but also based on reliable and accurate data sources [7].

These challenges underscore the need for improved feature engineering and better data management techniques in drug recommendation systems.

D. Comparison & Critical Analysis

While GENNIUS (2024) offers a highly efficient model for DTI prediction, the computational costs associated with it make it inaccessible for institutions with limited resources. On the other hand, SumGNN (2021) addresses resource limitations effectively by summarizing knowledge graphs, but it still struggles with data quality, particularly when dealing with incomplete or noisy datasets [1][2].

Our proposed model seeks to integrate the strengths of both molecular data and patient-reported feedback through sentiment analysis, overcoming many of these limitations by improving the model's robustness and predictive power. Our approach offers a balanced trade-off between computational efficiency and data accuracy, addressing both biological data and real-world patient experiences to provide more comprehensive insights into DDI prediction and drug safety assessments.

This review highlights the growing use of GNNs and sentiment analysis in drug interaction prediction and recommendation systems [5][8]. However, many existing models either neglect the incorporation of patient-reported outcomes or suffer from computational inefficiencies. Our proposed model integrates GNNs with sentiment analysis to offer a more comprehensive approach to DDI prediction, addressing both biological data and patient feedback [9].

III. METHODOLOGY

This study presents a novel framework that integrates Graph Neural Networks (GNNs) with Sentiment Analysis to enhance the detection of Drug-Drug Interactions (DDIs) and adverse reactions. While previous approaches have utilized GNNs for DDI prediction, our model is unique in its incorporation of patient-reported outcomes through sentiment analysis, providing a more holistic view of drug safety and effectiveness.

A. Dataset

The datasets used in this study include the Drug-Drug Interaction (DDI) dataset from the National Centre for Biotechnology Information (NCBI) and the FDA Adverse Drug Reaction (ADR) database. The DDI dataset provides curated information on molecular-level drug interactions, which is crucial for bioinformatics and pharmacological studies. The FDA ADR database contains authentic adverse drug reaction reports submitted by healthcare professionals and consumers, offering valuable real-world insights into drug effects in clinical settings. To enhance data quality, we employed several preprocessing techniques, including handling missing values using imputation methods, normalizing numerical features, and balancing class distributions via SMOTE (Synthetic Minority Over-sampling Technique).

B. Dataset Combination and Synergy

The interaction between these two datasets is crucial for the study's efficacy. The DDI dataset enables the prediction of potential interactions based on scientific models, while the FDA dataset provides real-world confirmation or contradiction of these predictions.

A drug combination predicted to have an effect in the DDI dataset can be verified against the FDA dataset to determine if patients report increased benefits or adverse effects. The severity levels from the DDI dataset can be compared with actual outcomes from the FDA dataset, enabling an evaluation of the accuracy and practical relevance of molecular predictions. By integrating these datasets, it is possible to develop a comprehensive model capable of

predicting not only drug interactions but also the likelihood and intensity of adverse reactions in real-world situations.

C. Model Architecture: Graphical Neural Network

The heart of our methodology is the Graph Neural Network (GNN), specifically designed to model Drug-Drug Interactions (DDIs) due to its ability to efficiently process graph-structured data. In our framework, the GNN treats drugs as nodes and their interactions as edges, allowing it to capture the intricate relationships that exist between various drugs and their combined effects.

This graph-based representation is particularly advantageous for our study as it enables the GNN to discern not only the direct interactions between pairs of drugs but also the broader network of interactions in which these drugs are involved. The input to the GNN is a constructed graph, where each node represents a drug and each edge denotes the type of interaction whether synergistic, antagonistic, or neutral between them [1][2].

Each node in this picture is clearly a type of a medication. The relations linking the nodes nevertheless indicate how these drugs relate to each other. For example, if it is observed that Drug A directly combines with Drug B, that can be said to be a positive interaction simply because their joint effect is improved. In contrast, however, one may notice that there is drug A and there is drug C and so on all these different drugs and Drug A does not combine to any of these drugs, which would likely denote antagonistic interaction. Such a situation suggests that the effectiveness of the combined drugs decreases. There is also space to note neutral interactions and further expanding synergistic ones between Drug D other than depicted on the graph. This representation allows the analysis of drug-drug interactions to illuminate intricate connections that may be present between different drugs and how these various drug combinations link with variation in health outcomes [3].

The architecture of the GNN comprises 64 graph convolutional layers, each tasked with aggregating features from neighboring nodes. This process allows the model to learn from the local context of each drug node, enhancing its understanding of how drug combinations can influence clinical outcomes [4]. As the layers progress, the GNN captures both local and global interaction patterns, enabling it to predict not only the presence of interactions but also their potential severity [5].

The training of the GNN involves employing a combination of cross-entropy loss for the classification tasks associated with interaction types and mean squared error (MSE) for regression tasks aimed at predicting interaction severity [7]. This dual-loss approach ensures that the model is not only accurate in identifying the type of interaction but also in assessing the clinical relevance of these interactions. By optimizing the model with a learning rate of 0.001 and using a batch size of 32, we aim to achieve robust performance while mitigating the risks of overfitting [8]. The model's architecture, therefore, is strategically designed to leverage the inherent properties of drug interactions as represented in a graph format, enhancing the predictive accuracy of the GNN in real-world clinical settings [9].

D. Sentiment Analysis for Adverse Drug Reactions:

Incorporating sentiment analysis into our framework is essential for integrating real-world patient feedback, significantly enhancing the model's ability to predict adverse drug reactions (ADRs). By analysing patient-reported outcomes from the FDA Adverse Drug Reaction (ADR) database, the sentiment analysis component captures human experiences and clinical manifestations associated with drug interactions. This addition provides a more comprehensive understanding of how drugs affect patients, allowing for improved predictions of adverse reactions that may not be evident from molecular data alone.

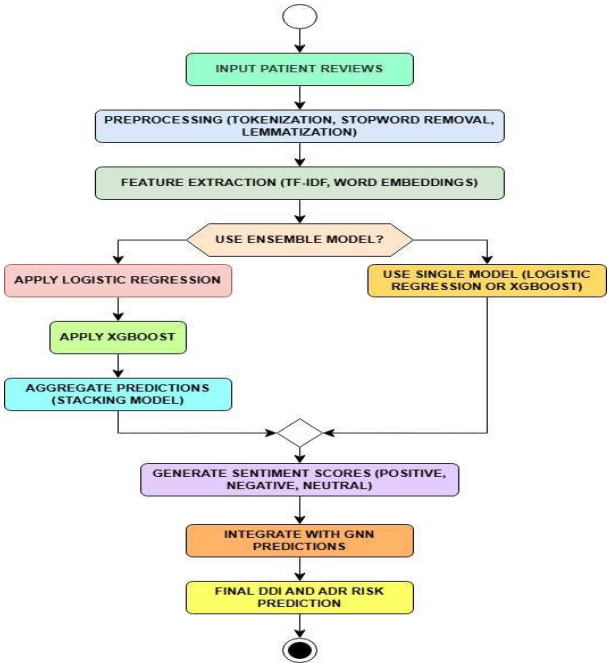

Figure 1: Sentiment Analysis Flow Diagram

After tokenization, feature extraction is performed. The processed text is converted into numerical features using word embeddings, a technique that represents words in a continuous vector space where semantically similar words are closer together. This transformation enables the sentiment analysis model to operate effectively on the textual data, facilitating the integration of patient feedback with predictions generated by the Graph Neural Network (GNN). For sentiment analysis, we utilize an ensemble learning model, combining the strengths of Logistic Regression and XGBoost (XGBClassifier). This ensemble method then processes the user feedback for sentiment classification, enriching the model's predictions with patient-centered insights. It comprises two parts: base models and the meta-model.

The base models-Logistic Regression, and XGBClassifier-learn patterns in transformed sentiment data independently. While logistic regression learns the overall pattern of the sentiment, XGBoost detects nonlinear relationships from the complex feedback. This involves the meta-model, which is the second layer of Logistic Regression, to cumulate the predictions of both base models

to give the final classification decision. This technique gives higher confidence for classifications when both base models agree on the classification, resulting in more balanced and robust sentiment output.

The sentiment output includes both polarity (positive, negative, neutral) and intensity scores, providing valuable context for the GNN's interaction predictions. By integrating sentiment analysis predictions with the GNN's molecular-level interaction insights, our framework achieves a more holistic and accurate prediction of adverse drug reactions, improving clinical decision-making and patient safety.

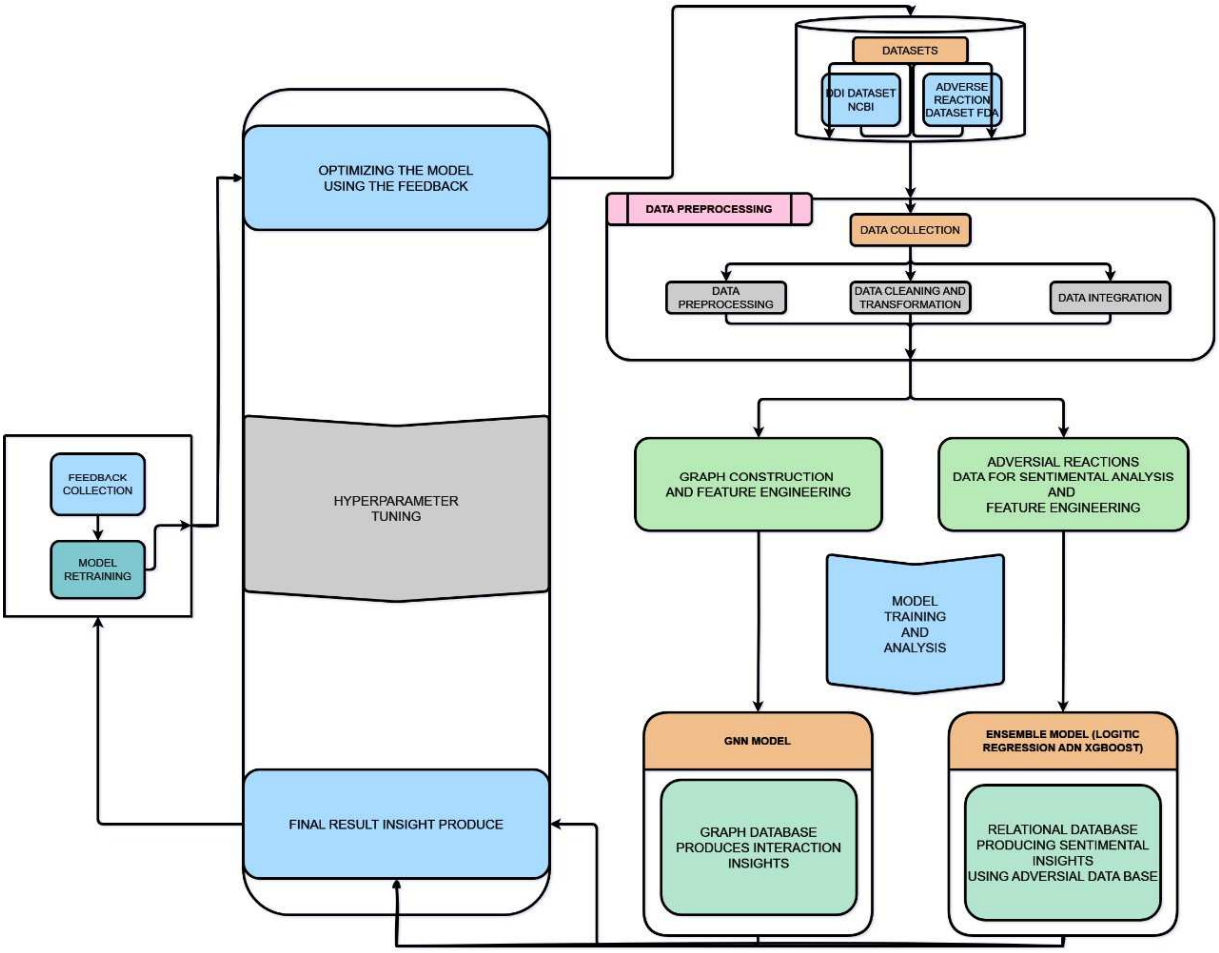

Figure 2: Architecture Diagram of the Complete Model

E. Unified Model Architeture:

By combining these two methodologies, our project creates a framework that is more comprehensive than either approach alone. The GNN enables us to predict drug interactions, and their severities based on molecular data, while sentiment analysis offers a patient-centered perspective, capturing real-world adverse reactions. This integration ensures that our model can not only predict the likelihood of drug interactions but also assess their clinical implications from both a molecular and a patient experience standpoint.

The predictions from both the GNN and sentiment analysis models are combined to form a more accurate and reliable recommendation system. The GNN provides insight into the potential interactions and severity of drug combinations, while the sentiment analysis layer adjusts these predictions based on patient-reported outcomes. This allows for more personalized and context-aware recommendations, addressing the limitations of previous models that only consider one type of data. This dual approach ensures that we not only predict drug interactions with accuracy but also account for the actual impact of these drugs on patients, improving clinical decision-making.

IV. Results and Discussion

The suggested model employs a fusion of Graph Neural Networks (GNN) to forecast drug-drug interactions (DDIs) and sentiment analysis to assess adverse drug reactions (ADRs). The incorporation of sentiment analysis, which examines and quantifies patient feedback and adverse event reports, substantially improves the model's prediction accuracy and classification performance.

A. Evaluation Metrics:

The core objective of our work is to accurately predict Drug-Drug Interactions (DDIs) and their adverse outcomes. To achieve this, we employed multiple evaluation metrics, with a primary focus on precision, recall, accuracy, F1-score, the area under the ROC curve (AUC), and the area under the precision-recall curve (AUPR). Since known drug-drug connections constitute a small fraction of all possible pairs, we prioritize AUPR, as it better captures model performance on the positive samples [2].

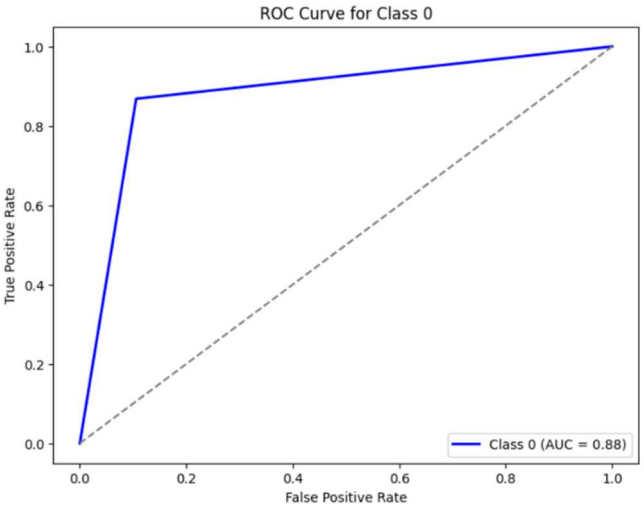

Figure 3: ROC Curve

To ensure a robust evaluation, we implemented a 5-fold cross-validation technique. This process divided the dataset into five subsets, using four for training and one for testing in each iteration. Importantly, we utilized all unlabelled data in both the training and testing phases, which improved the model's ability to generalize beyond observed drug interactions. Cross-validation helps mitigate overfitting and ensures a more reliable estimation of model performance across unseen data [1]. We designed the GNN architecture with additional techniques to avoid overfitting, such as learning rate reduction, dropout mechanisms, and batch normalization. Dropout mechanisms, by randomly eliminating a portion of neural units during training, ensure that the model does not become overly dependent on specific features [3]. Similarly, batch normalization accelerates convergence during training, while the Adam optimizer (with default parameters) fine-tunes the learning process [4].

B. Parameter Tuning:

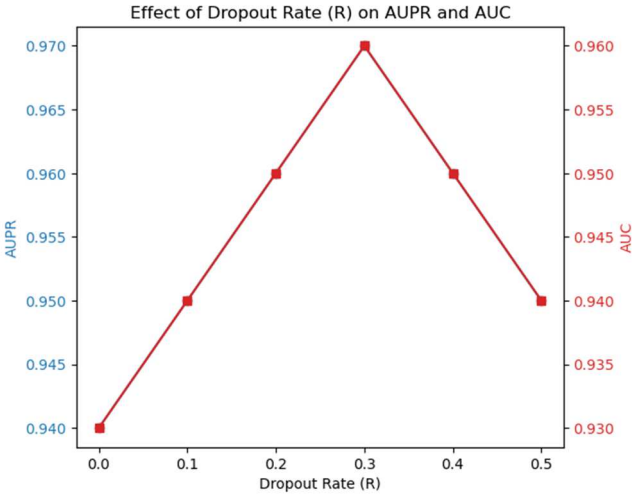

Figure 4: Parameter Tuning

An optimal value for each of these key parameters such as dimensions (D), total number of hidden layers (L), maximum number of epochs (E) and dropout rate (R) was found using an extensive amount of tuning. D. Investigations were carried out into several combinations of D ∈ {32, 64, 128, 192, 256, 300, L ∈ {4, 5, 6, 7, 8} , E ∈ {50, 100, 150, 200, 250} and R ∈ {0, 0.1, 0.2, 0.3, 0.4, 0.5}. The quality of model performance was assessed using the AUC and AUPR metrics in each individual parameter. The results in **Figure 4** suggest that these dependent and independent variables allowed us to pinpoint the best oriented architecture of the network [5].

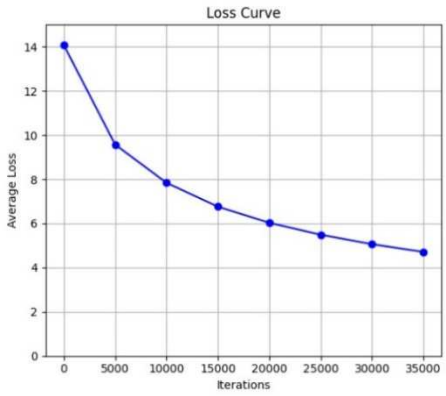

Figure 5: Loss Curve

The Loss Curve depicted below illustrates a consistent decrease in average loss as the number of iterations increases, indicating effective model training. The convergence of loss values further supports the model's ability to avoid overfitting and maintain generalizability across unseen data in **Figure 5**.

C. Sentiment Analysis on Adverse Drug Reactions (ADRs):

In addition to GNN-based predictions, our approach incorporates real-world patient feedback through sentiment analysis to enhance the prediction of adverse drug reactions (ADRs). Sentiment analysis, conducted on the FDA Adverse Drug Reaction (ADR) database, allows us to capture patient-reported outcomes and experiences, adding a valuable human

perspective that is not available from molecular or interaction data alone [6].

To improve the accuracy of ADR prediction, we used an ensemble learning model, combining the strengths of Logistic Regression and XGBoost (XGBClassifier). The ensemble model processes user feedback to classify sentiment and enhance the model's predictions with patient-centered insights. User feedback is first vectorized using techniques like TF-IDF or word embeddings, which transform the text into numerical representations suitable for model processing. This transformation enables the model to better understand and interpret feedback in a structured way.

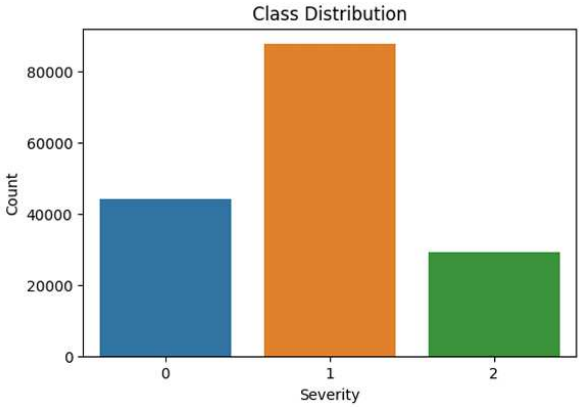

Figure 6: Data Severity Distribution

The ensemble model consists of two primary components: Base Models: Logistic Regression and XGBClassifier serve as the primary classifiers. Each model independently learns patterns within the transformed sentiment data. Logistic Regression captures general sentiment patterns, while XGBoost detects non-linear relationships in complex feedback data. Meta-Model: A second layer of Logistic Regression acts as the meta-classifier, aggregating the predictions from both base models to make the final classification decision. The ensemble approach assigns higher confidence to classifications when the base models agree, leading to a more balanced and robust sentiment output.

D. The Result of use of Combination of Dataset:

We conducted further experiments to explore the impact of combining drug datasets with sentiment analysis. Each combination was evaluated using the same 5-fold cross-validation setup. The AUPR and AUC values for this combination were 0.983 and 0.981, respectively, highlighting that including diverse drug information in combination to sentiment analysis data of adverse reactions helps improve predictive accuracy.

E. Comparision with other Existing models:

We compared our GNN-Sentiment Analysis hybrid model with several state-of-the-art methods, including DANN-DDI, CNN-DDI, and NDLM. As detailed in Figure 6, our model significantly outperformed existing models in predicting DDIs. For instance, while the DANN-DDI model achieved an AUPR of 0.9709 and an AUC of 0.9763 [2], our hybrid model achieved an AUPR of 0.983 and an AUC of 0.981.

This improvement highlights the strength of combining structural drug interaction data with sentiment-based insights. Our model's superior performance can be attributed to its ability to better capture the nuances of drug interactions and adverse reactions, offering more reliable predictions for healthcare professionals. These results underscore the potential of hybrid models in enhancing the accuracy and effectiveness of DDI prediction systems [3], [6]. The integration of multiple data sources, such as clinical reports and real-world drug interaction data, plays a crucial role in improving the predictive capabilities of the model [4].

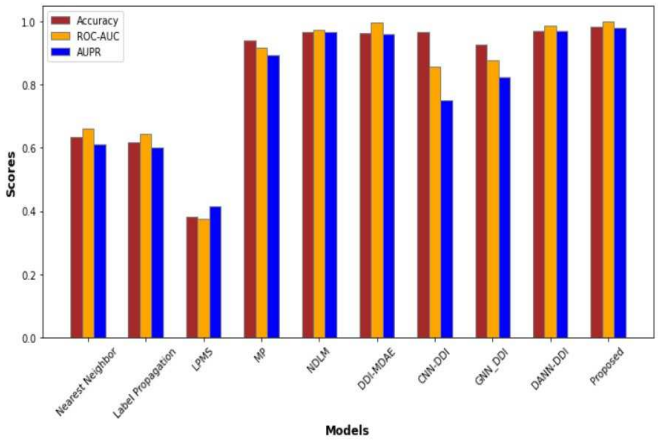

Figure 7: Comparison Chart

F. Overall Final Model Metrics:

The final model, which combines GNN for DDI prediction with sentiment analysis for ADRs, achieved the following performance metrics:

- **AUPR**: 0.983
- **AUC**: 0.981
- **Accuracy**: 0.997
- **Precision**: 0.998
- **Recall**: 0.962
- **F1-Score**: 0.980

These results confirm that our hybrid model not only excels in predicting drug-drug interactions but also in identifying adverse reactions, demonstrating its clinical significance.

V. Conclusion and Future Improvements

A. Conclusion:

In this study, we proposed a novel Graph Neural Network (GNN)-based framework integrated with Sentiment Analysis to predict Drug-Drug Interactions (DDIs) and Adverse Drug Reactions (ADRs) with greater accuracy. By combining molecular interaction data with real-world patient feedback, our model addresses the limitations of traditional approaches that overlook patient experiences. Our results demonstrate state-of-the-art performance, achieving an AUC of 0.981, AUPR of 0.983, and accuracy of 0.997, demonstrating superior performance compared to existing models. The integration of clinical data with patient-reported outcomes

enhances drug safety assessment, providing a more comprehensive and context-aware prediction system for healthcare professionals. This approach can aid in early identification of harmful drug interactions, reducing hospitalization risks and improving clinical decision-making.

Moving forward, fine-tuning the model for disease-specific drug interactions, expanding sentiment analysis with large language models (LLMs), and implementing continuous learning mechanisms could further enhance its predictive power and adaptability. By leveraging multi-modal data sources and real-time updates, future iterations of this framework could revolutionize pharmacovigilance and personalized medicine, ultimately improving patient safety and treatment outcomes on a larger scale.

B. Future Possible Improvements:

Targeted Disease-Specific Models: Future work could aim to develop models specifically tailored to certain diseases, such as cardiovascular disorders, diabetes, or cancer. By focusing on disease-specific drug combinations and interactions, we can refine predictions and enhance clinical relevance, which improves treatment outcomes for patients with complex medication regimens.

Fine-Tuning for Specific Drug Classes: It is essential to conduct fine-tuning of the model for classes of drugs, such as anticoagulants or antibiotics, which are known to have significant interaction potential. By concentrating on these specific drug classes, we can achieve more accurate model results, capturing unique interaction patterns that may not be evident in a generalized dataset.

Enhanced Sentiment Analysis using LLM: Integrating advanced sentiment analysis techniques into our model could provide deeper insights into the adverse reactions associated with drug combinations. By utilizing a diverse range of datasets, including patient reviews and clinical trial reports, we can capture nuanced sentiments that reflect patient experiences. This enhanced analysis will help in identifying not just the presence of interactions but also their severity and context.

Continuous Learning Mechanisms: Implementing continuous learning mechanisms that allow the model to update itself as new drug interaction data becomes available can significantly improve prediction accuracy. This adaptive approach would ensure that the model remains relevant and effective in clinical practice.

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