International Journal of Engineering Research and Science & Technology

Finding Adverse Drug Reaction Side Effects using Graph Neural

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Abstract: Adverse drug responses (ADRs) caused by drug-drug interactions are a major health concern. Graph Neural Networks (GNNs) are effective at modeling these relationships, but their one-dimensional processing limits their ability to extract complex features. This work offers a novel expansion that incorporates a two-dimensional Convolutional Neural Network (CNN2D) to enhance ADR prediction. By converting drug interaction data into 2D matrices and capturing intricate spatial connections, CNN2D improves the graph-based insights of the GNN. Our hybrid model performs better than more traditional methods like KNN and Decision Trees, with a prediction accuracy of 99.87%. The extension shows how deep learning might improve the evaluation of drug safety.

Index terms *- Adverse Drug Reactions, Drug-Drug Interactions, Graph Neural Networks, Convolutional Neural Networks, Self-Supervised Learning, SMILES Representation, Deep Learning, Side Effect Prediction, Drug Safety, TF-IDF Vectorization.*

1. INTRODUCTION

Pharmaceutical side effects known as adverse drug reactions (ADRs) can be unpleasant or hazardous and often require medical treatment, dosage adjustments, or discontinuing the medication completely. These reactions pose a serious threat to public health systems worldwide because they result in increased mortality, longer hospital stays, and a dramatic rise in healthcare costs. Since many adverse drug reactions (ADRs) are not found during clinical trials and only become apparent after the medication has been launched into the general market, early identification and prediction are essential.

Numerous variables, including as sex, geographic location, and healthcare quality, affect the prevalence of ADRs. For instance, studies show that women are more susceptible to adverse drug reactions (ADRs) due to pharmacokinetic and pharmacodynamic differences, as well as higher drug doses per body weight. Variations in medical standards and healthcare availability among countries may also have an influence on ADR reporting and management. Research indicates that a significant portion of ADRs—roughly 71.6% in wealthy nations and 59.6% in developing ones—can be prevented. The uniformity of ADR-related death rates across regions highlights the urgent need for effective forecasting techniques.

This study explores a deep learning-based approach that uses Graph Neural Networks (GNNs) and Self-Supervised Learning to anticipate drug-drug

interactions and the adverse effects associated with them in order to get around these challenges. By using structured representations of drugs and their interactions, the model aims to improve drug safety and save lives by increasing the accuracy of ADR diagnosis before medicines reach patients.

2. LITERATURE SURVEY

2.1 SSF-DDI: a deep learning method utilizing drug sequence and substructure features for drug–drug interaction prediction:

ABSTRACT: Background: Since combination treatment frequently results in drug-drug interactions (DDI), it's critical to recognize and be ready for any DDI. Many AI techniques may be able to anticipate and identify possible DDI, however they often ignore drug molecule sequence information and the role that molecular substructures play in DDI. Results To address these problems, we developed a new sequence and substructure feature-based DDI prediction model (SSF-DDI) in this study. In order to provide a more thorough and accurate representation of drug molecules and to provide better information for DDI prediction, our model incorporates structural and drug sequence data from the drug molecule graph. In summary, trials and case studies have shown that SSF-DDI significantly outperforms the most advanced DDI prediction models in a variety of actual datasets and scenarios. SSF-DDI outperforms state-of-the-art techniques in predicting DDI using unknown drugs, improving accuracy by 5.67%.

2.2 Modular Multi-Source Prediction of Drug Side-Effects With DruGNN:

ABSTRACT: Drug development procedures, public health, and healthcare system expenses are all significantly impacted by drug side effects, or DSEs. Reducing this impact, especially on drug research, requires anticipating potential harmful effects before they materialize. Candidate molecules could be examined before to clinical trials, saving participants' time, money, and health. Drug structures and protein-protein interactions are only two examples of the complex biological mechanisms that lead to medication side effects. Data from several sources must be merged in order to forecast their occurrence. This study expressively expresses the relationship information between various things, such as genes and pharmacological drugs, by merging such separate data into a network dataset. One significant development for pharmaceutical side-effect predictions is the dataset's relational structure. With extremely encouraging findings, we use Graph Neural Networks (GNNs) to forecast DSEs on our dataset. Deep learning models, such as GNNs, have been used in many biological applications because they can understand graph-structured data with little information loss. Our experimental findings confirm the benefits of taking use of connections between data items and offer encouraging paths for further advancements in this area. The experiment also demonstrates the significance of particular data subsets in identifying drug-side effect connections.

2.3 Explainable Drug Repurposing Approach From Biased Random Walks:

ABSTRACT: The goal of the very busy area of drug repurposing research is to find new uses for

medications that have previously been produced for a range of therapeutic objectives. Every approach has its own benefits, and even with the advancement of protocols, success is still only partially achieved. We provide a new approach in this composite situation based on reliable drug-gene-disease correlation data sets, with an emphasis on an effective mathematical process based on gene similarity scores and biassed random walks. The Markov chain underlying the random walk process further reveals the recommendation mechanism, making it possible to comprehend how the outcomes are proposed. When compared to the state-of-the-art in pharmaceutical repurposing methodologies, performance evaluation and analysis of a case study on rheumatoid arthritis demonstrate that our methodology is computationally efficient and accurate in offering helpful recommendations.

2.4 A Novel Drug-Drug Indicator Dataset and Ensemble Stacking Model for Detection and Classification of Drug-Drug Interaction Indicators:

ABSTRACT: Drug-drug interactions (DDI) occur for more than 30% of unexpected clinically dangerous pharmacological events, making them a significant public health concern. Research on informatics-based DDI signal detection has advanced within the last ten years. The goal of this study is to develop an ensemble stacking machine learning (ML) approach that can reliably predict novel DDI hazard indicators. One of the best pharmacological data sources, DrugBank, supports the stacking ensemble machine learning architecture to predict the signals of drug-drug interactions. We make a sizable collection of drug-related information, such as names, kinds, and other elements of drug indicators, freely accessible to the scientific community. Data preparation, label encoding and one hot encoding for categorical variables, balancing by random oversampling, and ensemble stacking for model prediction are all part of the suggested technique. The suggested ensemble method classifies the pharmaceutical indication classes using Gaussian Naive Bayes (GNB), Adaboost, and the Gradient Boosting (GB) classifier. The experiment's findings show that the recommended strategy works more accurately and efficiently than conventional machine learning techniques. At 99.0%, the stacking model achieved the maximum accuracy. The test shows that the suggested model outperforms conventional techniques in identifying signs of drug interactions.

2.5 NNDSVD-GRMF: A Graph Dual Regularization Matrix Factorization Method Using Non-Negative Initialization for Predicting Drug-Target Interactions:

ABSTRACT: The process of creating and developing novel drugs can be greatly accelerated by accurately predicting drug-target interactions (DTIs). A variety of matrix factorization techniques have been used in recent years to predict DTIs. However, their convergence and performance cannot be guaranteed because the majority of them rely on heuristic and iterative approaches. Dual graph regularization Non-negative matrix factorization (GDNMF) and non-negative double singular value decomposition (NNDSVD) serve as the foundation for our novel technique, NNDSVD-GRMF. By taking into account both the initialization step of the non-negative matrix factorization and the structural information of the data and features, it properly predicts DTIs. The NNDSVD-GRMF extension (NNDSVD-WGRMF) is also suggested to enhance the algorithm's flexibility.

Our methods outperform existing state-of-the-art procedures, according to extensive experimental data. Nine of the ten medications that were anticipated to interact with the androgen receptor based on the case studies have also been verified, along with nine of the ten target proteins that nicotine bitartrate was projected to target.

3. METHODOLOGY

i) Proposed Work:

The proposed system enhances Adverse Drug Reaction (ADR) prediction by integrating a Graph Neural Network (GNN) architecture with a two-dimensional Convolutional Neural Network (CNN2D). While the GNN employs graph structures to capture intricate drug-drug interactions, the CNN2D extension transforms drug feature data into a two-dimensional format to extract sophisticated spatial patterns. This hybrid model significantly increases prediction accuracy by utilizing CNN2D's advanced feature extraction capabilities, achieving an incredible accuracy of 99.87%. The technology offers a more sophisticated and dependable way to detect potential side effects, improve drug safety, and assist medical professionals in making educated decisions.

ii) System Architecture:

The first steps in designing the proposed system are data preparation and collecting. SMILES strings, which stand for chemical structures, drug IDs, and known side effects are all included in the collection, which is sourced from DrugBank. These SMILES texts are converted into numerical vectors to be utilized as input for model training. TF-IDF vectorization is used to extract important features from textual input and decrease noise from frequent words. The data is separated into training and testing sets after processing. A Graph Neural Network (GNN), where each medicine is represented as a node and its interactions as edges, is initially used to describe the complex relationships between pharmaceuticals. This graph-based model does a good job of capturing drug dependency patterns.

To further enhance the prediction capabilities, a two-dimensional Convolutional Neural Network (CNN2D) is introduced. By analyzing the same data in a 2D matrix form, CNN2D enables the model to extract spatial features that are not available through traditional graph topologies. This deep learning model's enhanced capacity to recognize hidden patterns and interactions leads to higher prediction precision. A Flask-based user interface allows administrators to easily visualize forecasts and submit test results. CNN2D for complex pattern recognition and GNN for structural learning are combined to build a powerful hybrid system that can accurately identify potential adverse pharmaceutical reactions before they manifest clinically.

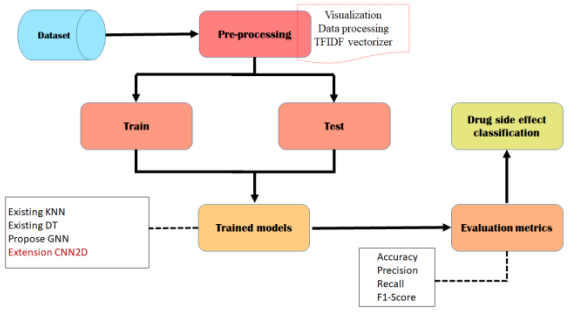

Fig.1. Proposed Architecture

iii) MODULES:

- **Data loading:** We will import the dataset using this module.

- **Visualization:** Side effect frequencies are clearly represented by the visualisation, which shows a graph with different Side-Effects IDs along the x-axis and their matching record counts on the y-axis.
- **Data Pre-processing:** Quantitative analysis is made easier by converting the drug data into numeric vectors. The generated vector values are then shown for additional processing in order to train machine learning models.
- **TFIDF Vectorization:** By determining term frequency and inverse document frequency, TFIDF vectorisation turns textual drug data into numerical representations, highlighting pertinent phrases and lessening the influence of frequent words in the dataset.
- **Splitting data into train & test:** Data will be separated into train and test using this module.
- **Model generation:** Model, Current KNN, Current Decision Tree, Suggested GNN, and CNN2D Extension. Each algorithm's performance assessment metrics are computed.
- **Admin login:** This module allows the administrator to log in.
- **Drug Side Effect Prediction:** This module allows users to upload test data.
- **Prediction:** The final prediction was shown.

iv) ALGORITHMS:

a) K-Nearest Neighbors (KNN)

The K-Nearest Neighbors (KNN) method is a simple instance-based learning strategy that organizes data points based on the majority class of their closest neighbors. KNN is employed in our attempt to predict unfavorable medication reactions by looking at similarities between pharmacological properties and previously reported side effects. Because of its ease of use, it is a good place to start when comparing to more complex algorithms and creating a benchmark for evaluating performance.

b) Decision Tree

The Decision Tree approach builds a model with a tree-like structure to provide judgments based on feature values. In our study, it is utilized to classify drugs and predict side effects by creating branches that represent several decision paths based on drug properties. Because decision trees offer interpretability, which allows stakeholders to understand the reasoning behind projections, they are useful for analyzing complex drug interactions and their potential negative effects.

c) Graph Neural Network (GNN) (Proposed)

The proposed Graph Neural Network (GNN) uses graph topologies to mimic drug-drug interactions and predict undesirable reactions. By representing interactions as edges and drugs as nodes, the GNN is able to capture complex correlations in the data. The GNN in our study examines pharmacological features expressed as numerical vectors to identify patterns and relationships and provide accurate predictions of potential side effects. This innovative approach addresses the shortcomings of traditional algorithms while increasing forecast accuracy.

d) Convolutional Neural Network 2D (CNN2D) (Extension)

The Convolutional Neural Network (CNN2D), a deep learning technique, excels in extracting spatial information from two-dimensional input. Our work uses CNN2D to increase the prediction capability of

drug-drug interaction studies. By transforming drug data into a two-dimensional representation, CNN2D learns intricate patterns that aid in the detection of potential adverse reactions. This algorithm outperforms the GNN's results and makes more accurate side effect predictions by employing advanced feature extraction techniques.

4. EXPERIMENTAL RESULTS

The experimental findings were obtained using the DrugBank dataset, which includes drug IDs, SMILES strings, and the associated side effects. Numerous models were compared and assessed based on prediction accuracy. Conventional methods such as K-Nearest Neighbors (KNN) and Decision Tree have 91% and 95% accuracy, respectively. The proposed Graph Neural Network (GNN), which effectively captures complex drug-drug relationships, increased the accuracy to 97.69%. To further enhance performance, a CNN2D model was added; it achieved the best accuracy of 99.87% and recovered spatial information. These results show how effectively the GNN-CNN2D approach forecasts unfavorable drug reactions.

Accuracy: A test's accuracy is determined by its capacity to distinguish between healthy and ill cases. To gauge the accuracy of the test, find the percentage of examined instances that had true positives and true negatives. According to the computations:

Accuracy = TP + TN /(TP + TN + FP + FN)

$$Accuracy = \frac{(TN + TP)}{T}$$

Precision: Precision is the number of affirmative cases or the classification's accuracy rate. The following formula is applied to assess accuracy:

Precision = True positives/ (True positives + False positives) = TP/(TP + FP)

$$\Pr e\,cision = \frac{TP}{(TP + FP)}$$

Recall: A model's ability to recognise every instance of a pertinent machine learning class is measured by its recall. The ratio of accurately predicted positive observations to the total number of positives indicates how well a model can identify class instances.

$$Recall = \frac{TP}{(FN + TP)}$$

mAP: Mean Average Precision is one ranking quality metric (MAP). It considers the number of relevant recommendations and their position on the list. MAP at K is calculated as the arithmetic mean of the Average Precision (AP) at K for each user or query.

$$\boldsymbol{mAP = \frac{1}{n}\sum_{k=1}^{k=n} AP_k}$$

$$\boldsymbol{AP_k = \text{ the AP of class } k}$$

$$\boldsymbol{n = \text{ the number of classes}}$$

F1-Score: An accurate machine learning model is indicated by a high F1 score. combining precision and recall to increase model correctness. The accuracy statistic quantifies the frequency with which a model correctly predicts a dataset.

$$F1 = 2 \cdot \frac{(Recall \cdot \Pr e\,cision)}{(Recall + \Pr e\,cision)}$$

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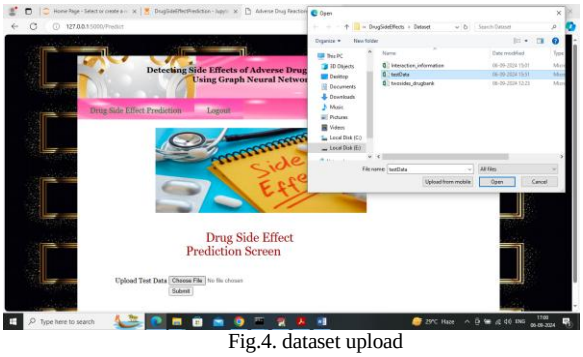

Fig.4. dataset upload

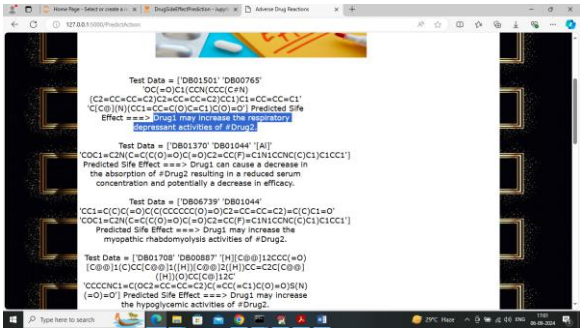

Fig.5. results

	Algorithm Name	Accuracy	Precision	Recall	FSCORE
0	Existing KNN	91.560102	91.920962	91.305660	91.323465
1	Existing Decision TRee	95.140665	95.339149	95.618899	95.454287
2	Propose GNN	97.698210	97.889953	97.702843	97.722705
3	Extension CNN2D	99.872123	99.903101	99.888143	99.895292

Fig.6.accuracy table results

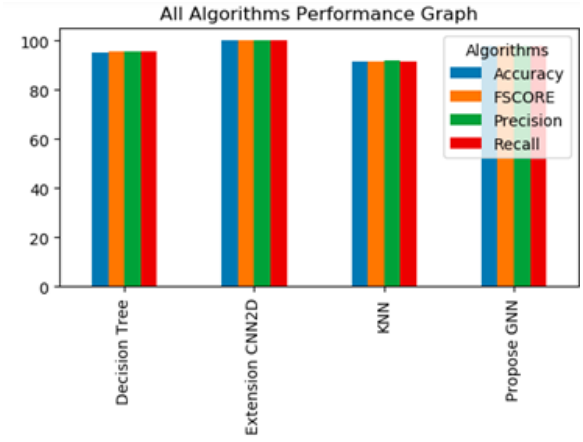

Fig.6. graphical representation

5. CONCLUSION

The results of the study demonstrate the critical need for a trustworthy and effective technique to forecast adverse drug reactions (ADRs), a significant public health concern brought on by drug interactions. Because they depend too heavily on post-marketing data and are unable to discover uncommon interactions before to a drug's distribution, current detection techniques frequently fail. Our suggested approach, which combines Self-Supervised Learning with a Graph Neural Network (GNN), has a notable capacity to predict possible ADRs. The GNN greatly improves the prediction process by capturing the intricate linkages that might result in negative responses by efficiently modeling the interactions between medications. The GNN surpasses conventional algorithms with an astounding accuracy of 97.69%, demonstrating its efficacy in identifying potentially hazardous medication combinations. Performance is further improved by using cutting-edge techniques, such as a two-dimensional Convolutional Neural Network (CNN2D), which achieves an incredible accuracy of 99.87%. This study shows how advanced machine learning methods may be applied to enhance patient outcomes and medication safety, which will ultimately lead to better healthcare practices and a decrease in the frequency of adverse drug reactions.

6. FUTURE SCOPE

In order to improve prediction accuracy and model resilience, the future scope of this project will examine combining cutting-edge methods including ensemble learning, reinforcement learning, and transfer learning. The system's capacity to recognize intricate drug-drug interactions may potentially be

enhanced by including more varied datasets and employing unsupervised learning strategies. In order to reveal the model's decision-making process and promote mutual respect and understanding among medical experts, it will also be essential to analyze the application of explainable AI approaches.

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