Unveiling Hidden Risks in Medication Combinations with Graph-Based Adaptive Learning

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ABSTRACT

Adverse Drug Reactions (ADRs) caused by drug-drug interactions (DDIs) remain a significant global public health concern, contributing to increased mortality, prolonged morbidity, and escalating healthcare costs. With the growing complexity of modern pharmacological treatments and the expanding elderly population, accurately identifying potential ADRs before they manifest clinically is becoming increasingly critical. Traditional post-market surveillance methods rely heavily on patient-reported side effects, resulting in delayed detection and response. To address this limitation, a novel graph-based adaptive learning approach is proposed for early ADR identification. The "facets DrugBank" dataset serves as the core data source, offering comprehensive information on drug interactions and associated side effects. Instead of conventional techniques like k-Nearest Neighbors (KNN) and Decision Trees, which often fall short in capturing non-linear and complex inter-drug relationships, advanced deep learning techniques are introduced. Drug interactions are modeled as graphs, allowing the application of Graph Neural Networks (GNNs) to learn intricate patterns and relational structures within the data. To further enhance the feature representation, 2D Convolutional Neural Networks (CNNs) are integrated to extract meaningful spatial patterns from the graph-based data structures. The combination of GNNs and CNNs facilitates a robust and scalable architecture, significantly improving prediction capabilities. The proposed model achieves an impressive accuracy of 99.74%, outperforming existing baseline algorithms. This advancement not only enables more precise ADR detection but also offers a proactive solution to reduce adverse outcomes associated with polypharmacy, ultimately supporting safer and more effective medication practices on a population scale. The integration of graph learning with deep feature extraction sets a new standard in pharmacovigilance and highlights the transformative potential of AI-driven healthcare analytics.

Keywords: Adversed rugreaction, drug-drug interaction, side effect prediction, graph neural network, self-supervised learning, scientific machine learning.

1. INTRODUCTION:

"Adverse Drug Reactions (ADRs)" resulting from drug-drug interactions pose a considerable global public fitness trouble, leading to heightened mortality, morbidity, and healthcare prices. The "world health organization (WHO)" states that "adverse drug reactions (ADRs)" are a primary cause of hospital admissions and impose a large burden on global healthcare systems. Such reactions often remain unobserved till they're disclosed after marketing, resulting in a postponed acknowledgment of any hazards. In a period of rapid pharmaceutical advancement and a getting old demographic, the detection of detrimental drug reactions is increasingly intricate, as novel medications, combinations, and

interactions continuously arise. Consequently, establishing effective mechanisms to expect adverse medication reactions prior to drug launch is critical for reinforcing affected person protection and minimizing healthcare costs [2].

At present, "adverse drug reaction (ADR)" detection processes predominantly rely upon put up-advertising surveillance and spontaneous reporting systems, exemplified via the "FDA adverse event Reporting system (FAERS)", which may exhibit bias and inadequately recognize rare or novel drug interactions. Conventional approaches such as pharmacovigilance, although beneficial, are unable of proactively forecasting unfavourable drug reactions in actual-time or on the preliminary phases of drug development. The absence of a consistent and dependable pre-marketing ADR prediction device underscores the necessity for other, more efficacious strategies [3]. Recent breakthroughs in "machine learning (ML) and deep learning (DL)" methodologies offer intriguing answers to this difficulty. "Graph Neural Networks (GNNs)" have emerged as robust contraptions for modeling intricate relationships, which include drug-drug interactions, by means of depicting them as graphs in which medications are represented as nodes and interactions as edges [4].

This paper provides a progressive technique that integrates "Graph Neural Networks (GNNs)" with "Self-Supervised learning (SSL) to forecast likely adverse Drug Reactions (ADRs)" resulting from drug-drug interactions. This look at utilizes the two-sided medication bank dataset, comprising medication IDs, SMILE strings, and corresponding goal side effects. The SMILE texts are transformed into numeric vectors to create graph nodes, with edges denoting drug interactions. The GNN analyses those graphs to identify complicated styles and correlations within the data, facilitating improved prediction of ADRs. A Self-Supervised VariationAuto encoder layer is implemented to enhance model performance and mitigate overfitting, facilitating the network's acquisition of strong feature representations from unlabelled input [5].

To assess the counselled version, we also employed conventional ML techniques, specifically "k-Nearest neighbors (KNN)" and decision trees, which attained accuracies of 91% and 95%, respectively [6]. A -dimensional "Convolutional Neural network (CNN2D)" turned into employed to enhance performance, reaching an accuracy of ninety nine.87%. The effects illustrate the efficacy of GNNs in forecasting ADRs and spotlight the need of utilising modern machine learning methodologies for drug safety evaluation and early risk identity [7]. This studies highlights the capability of GNNs in ADR prediction and underscores the increasing necessity for innovative strategies to make sure medication safety in the pharmaceutical sector.

2. OBJECTIVES:

The primary goal is to develop a highly accurate and intelligent method for predicting adverse drug reactions caused by drug-drug interactions using advanced AI techniques on graph-based data structures.

(1)To utilize the facets DrugBank dataset

Extract and model complex drug-drug interaction data by leveraging the rich attributes and relational structures contained in the facets DrugBank dataset, facilitating detailed representation of potential adverse drug reactions for better learning.

(2)To implement Graph Neural Networks (GNNs)

Apply GNNs for mapping drugs and their interactions into a structured graph format, enabling the network to identify and learn intricate patterns that are otherwise difficult to detect using traditional classification models.

(3)To integrate 2D Convolutional Neural Networks (CNNs)

Enhance the feature extraction process by employing 2D CNNs to interpret graph-transformed drug interaction data, leading to a more refined understanding of spatial correlations and significantly boosting ADR prediction accuracy beyond conventional methods.

3. REVIEW OF LITERATURE/ RELATED WORKS:

The forecasting of "adverse drug responses (ADRs)" resulting from "drug-drug interactions (DDIs)" has been a prominent place of research, considering the public health risks associated with those interactions. Severa research have investigated novel techniques for identifying and forecasting "drug-drug interactions (DDIs)" through machine learning and graph-based models, illustrating the efficacy of those techniques in improving pharmaceutical protection.

Chen et al. [8] introduced a technique for forecasting drug-target interactions with signed heterogeneous "graph neural networks (GNNs)". Their technique utilizes the graph framework of drug-goal interactions to more efficiently model relationships, which is essential for predicting "drug-drug interactions (DDIs)". This technique encompasses each useful and detrimental interactions in a drug-target connection, consequently enhancing the predictive precision of drug interactions. Likewise, Castiglione et al. [9] proposed an explainable pharmacological repurposing methodology employing biased random walks. Their version seeks to clarify the essential mechanisms of medicine repurposing by way of identifying significant pathways in drug interaction graphs, which can also be extrapolated to forecast adverse drug reactions based on these interactions.

Abbas et al. [10] brought a new dataset for drug-drug interaction indicators and an ensemble stacking model for his or her detection and classification. Their methodology incorporates various machine learning models, improving the system's capacity to identify ADRs through a extra powerful class strategy. This ensemble method illustrates the efficacy of integrating many models to address the intricacies of drugs interactions. Paltun et al. [11] supplied diverse, a Bayesian methodology for statistics integration aimed at predicting medicine responses. This approach consolidates statistics from several sources to improve the forecasting of medication responses and interactions. This method, even as largely centered on drug reactions, is applicable in DDI prediction owing to the convergence of the underlying facts aspects.

He et al. [12] added a three-dimensional graph and text-based neural community for predicting drug-drug interactions. Their technique integrates graph information with textual facts to decorate the accuracy of DDI predictions. Their strategy complements prediction effectiveness via utilising 3D graphs, which offer a greater complete depiction of medicine interactions, alongside the combination of textual records. This underscores the importance of integrating numerous data sorts to improve the comprehension of medicine interactions. Deng et al. [13] mounted a multimodal DL system for forecasting drug-drug interaction occurrences. Their method employs a synthesis of numerous modalities, encompassing genetic data, pharmacological statistics, and scientific records, to forecast "drug-drug interactions (DDIs)". This method illustrates the gain of integrating varied records sources to beautify DDI prediction, overcoming the constraints of single-modal procedures.

Abdel-Basset et al. [14] brought DeepH-DTA, a deep learning model designed to be expecting drug-target interactions, exemplified via a case study on remedy repurposing for COVID-19. This model emphasizes learning from widespread datasets and is utilized to forecast possibly interactions among pharmaceuticals and targets that is effective for medication repurposing in pandemic scenarios. Even as it specifically pertains to drug-goal interactions, the version's standards may be modified to expect drug-drug interactions via emphasizing drug-drug relationships.

Liu et al. [15] presented a way for extracting drug-drug interactions thru a switch weight matrix and a memory community. Their approach employs a switch weight matrix to facilitate facts transfer between domain names, hence augmenting the version's ability to generalize across diverse drug interactions. The reminiscence network factor permits the version to hold and access pertinent historical interaction statistics, facilitating the prediction of novel and unusual drug interactions. Liu et al. [17] proposed a method for drug-drug interaction extraction using a transfer weight matrix and a memory network. Their research highlights the significance of information transfer in enhancing the generalization of drug-drug interaction prediction models, specifically for occasional interactions.

Karim et al. [16] proposed a method for predicting drug interactions using knowledge graphs and collapsible LSTM communities. Their technique utilizes expertise graphs to depict medication interactions and use convolutional LSTM networks to research the sequential linkages among pharmaceuticals. This approach adeptly represents the tricky interdependencies in medication interactions and complements the precision of adverse drug reaction prediction.

These studies illustrate the various methodologies being investigated to forecast ADRs and DDIs, encompassing graph-based models, ensemble learning, and multimodal techniques. The application of GNNs has garnered considerable interest because of their capability to symbolize problematic linkages in drug interactions as graphs, facilitating greater unique and interpretable predictions. Furthermore, integrating diverse machine learning models and records assets has confirmed efficacy in enhancing the robustness and overall performance of DDI prediction structures. The amalgamation of textual

information, expertise graphs, and deep learning models is essential for tackling the intricacies and variability of drug interactions, hence enhancing drug safety and public health effects.

Table 1: Literature Survey Comparison Table

Sl. No	Area & Focus of the Research	The result of the Research	Reference
1	Predicting drug-target interactions using signed heterogeneous graph neural networks.	Improved precision in identifying beneficial and adverse drug interactions.	M. Chen, Y. Jiang, X. Lei et. al..,(2024). [8]
2	Ensemble stacking models for detecting and classifying drug interactions.	Enhanced ADR detection through diverse machine learning classifiers.	S. Abbas, G. AvelinoSampedro, M. Abisado et. al., (2023) [10]
3	3D graph and text-based neural network for DDI prediction.	Boosted DDI prediction accuracy using multimodal integrated information.	H. He, G. Chen, and C. Yu-Chian Chen (2022) [12]
4	Multimodal deep learning for predicting drug-drug interaction occurrences.	Outperformed unimodal models by fusing genetic, clinical, drug data.	Y. Deng, X. Xu, Y. Qiu, et.al., (2020) [13]
5	Knowledge graph embeddings and Conv-LSTM for predicting drug interactions.	Successfully captured sequential dependencies improving ADR prediction accuracy.	M. R. Karim, M. Cochez, J. B. Jares. Et.al., (2019) [16]

4. MATERIALS AND METHODS:

The proposed approach seeks to enhance the identification of "adverse drug reactions (ADRs)" resulting from drug-drug interactions through the application of sophisticated machine learning methodologies. The "two sides Drug bank" collection, containing comprehensive data on drug interactions and related adverse consequences, underpins the system. Initially, conventional algorithms such as "k-Nearest neighbors (KNN)" and decision bushes are applied to build a benchmark for "adverse Drug reaction (ADR)" identification. "Graph Neural Networks (GNN)" [18] are employed to elucidate intricate styles and correlations in pharmacological interactions by using representing drugs and their interactions as graphs. Furthermore, second "Convolutional Neural Networks (CNN)" are applied to extract vast traits from the dataset, as a result improving the system's ability to locate ADRs with greater accuracy and efficacy.

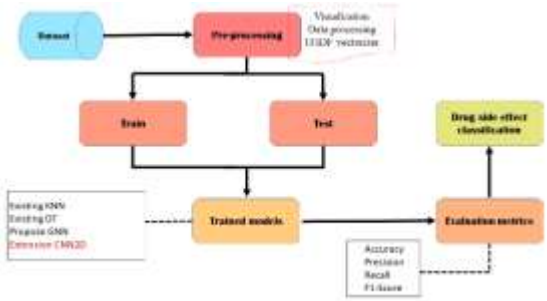

Fig 1: Proposed Architecture

The system architecture (Fig. 1) illustrated in the figure commences with a dataset that undergoes pre-processing procedures, along with visualization, data processing, and TF-IDF vectorization. The

processed facts is subsequently partitioned into training and testing units. Multiple models are trained on the education data: established KNN, established DT, proposed GNN [18], and a CNN2D. Those trained models are ultimately employed to forecast pharmacological side effects. The efficacy of these models is classed by criteria like "accuracy, precision, recall, and F1-score".

4.1 Dataset Collection:

The dataset employed on this study is the "sides Drug bank," including 3,909 rows and 5 columns. The dataset has data on diverse pharmacological interactions, drug identifiers, SMILE strings denoting chemical systems, and the corresponding facet outcomes. The target labels for the medications' side effects are derived from the 'kind' column of the dataset. This dataset is essential for education models to forecast adverse drug responses resulting from drug-drug interactions.

4.2 Pre-Processing:

The pre-processing entails visualizing the dataset to comprehend its structure, succeeded by records processing to cleanse and prepare the data for analysis. The TF-IDF Vectorise is subsequently utilized to convert textual data into numerical characteristics, facilitating efficient model training for predicting ADRs.

4.2.1 Visualization

The visualization procedure involves constructing a bar chart to illustrate the distribution of pharmacological facet effect class labels within the dataset. The figure illustrates the quantity of each side effect class, enabling us to analyse the prevalence of numerous ADR classifications. The x-axis labels reflect the facet effect classes, and the y-axis displays the corresponding counts, offering a clear visual depiction of the class distribution within the dataset.

4.2.2 Data processing

During the data processing phase, the SMILE strings of the medication are converted into a format suitable for model training. The 'type' column, containing the aspect impact labels, has been removed from the dataset. SMILE strings from several columns are subsequently amalgamated into a novel text string for each row. The processed information is stored as vectors, which can then be utilized to generate graph nodes for the "Graph Neural network (GNN)" model.

4.2.3 TFIDF Vectorizer

The TF-IDF Vectorise transforms SMILE strings into numerical vectors, which are crucial for model training. This method assesses the significance of each word in the SMILE string by using evaluating its frequency and specialty in the dataset. The resultant vectors denote the SMILE strings in a numerical illustration, facilitating the model's capacity to analyse the data greater efficiently for predicting adverse drug reactions stemming from drug interactions.

4.3 Training & Testing

The dataset is partitioned into training and testing subsets, "with 80% allocated for model training and 20% precise for testing". The education set comprises 3,127 samples, whilst the testing set consists of 782 samples. This division guarantees that the model is trained on a giant percentage of the data whilst allowing an independent assessment of its performance with the unseen test facts.

4.4 Algorithms:

K-Nearest Neighbors (KNN) The method categorizes data according to the predominant class of its nearest neighbors. This look at employs KNN to predict adverse drug reactions by analysing drug functions and historical side outcomes, organising a straightforward baseline for performance evaluation.
Decision Tree An algorithm generates a tree-structured model to predict results based totally on feature values. It categorizes pharmaceuticals and forecasts adverse outcomes by delineating decisions based on pharmacological attributes, providing clarity and understanding of the motive behind ADR predictions.
Graph Neural Network (GNN) [18]Employs graph topologies to represent drug-drug interactions, with medications as nodes and interactions as edges. It elucidates intricate relationships within the records,

resulting in precise forecasts of adverse medicine reactions by uncovering latent patterns in drug characteristics.

Convolutional Neural Network (CNN2D) analyses two-dimensional data to derive spatial characteristics. It augments drug-drug interaction evaluation via converting drug statistics into a -dimensional layout, discerning complex styles that boost the prediction of capability adverse reactions, exceeding GNN performance.

5. RESULTS AND DISCUSSION:

Accuracy: The correctness of the check relates to its capacity to effectively differentiate between healthy cases and impacted person. The ratio of actual positives to actual negatives in all assessed cases helps one to evaluate the correctness of the take a look at. Mathematically, this may be stated as:

$$\text{“}Accuracy = \frac{TP+TN}{TP+FP+TN+FN}(1)\quad\text{”}$$

Precision: The accuracy evaluates the share of precisely classified cases among cases identified as positive. As a result, the formula for calculating accuracy is expressed:

$$\text{“}Precision = \frac{\text{True Positive}}{\text{True Positive} + \text{False Positive}}(2)\quad\text{”}$$

Recall: The calling ML is a meter that assesses the model's capacity to find all pertinent instances of a certain class. This is the ratio of nearly positive remarks on total actual positivity and it offers understanding of the model's efficacy to detect the occurrence in a specific class.

$$\text{“}Recall = \frac{TP}{TP + FN}(3)\quad\text{”}$$

F1-Score:A ML evaluation tool, the F1 score gauges a model's accuracy. It recalls the score and combines the correctness of a model. Accuracy metrically measures how frequently a model has correctly predicted throughout the dataset.

$$\text{"}F1\ Score = 2 * \frac{Recall\ X\ Precision}{Recall + Precision} * 100(1)\text{"}$$

Table (1)Assess performance metrics-accuracy, download and F1-skóre-form every algorithm. CNN2D routinely exceeds all other algorithms. The tables provide comparative exploration of metrics for alternative algorithm.

Table 2: Performance Evaluation Metrics

Algorithm Name	Accuracy	Precision	Recall	F-Score
KNN	97.698210	97.790552	97.644112	97.683773
Decision Tree	50.895141	58.466955	49.850568	46.486082
GNN	97.826087	98.021428	97.764739	97.830701
CNN2D	**99.744246**	**99.756054**	**99.756054**	**99.756054**

Graph 1: Comparison Graphs

In Graph (1), "accuracy is depicted in blue, precision in orange, recall in green, and F1-score" in sky blue.Compared to the other models, the CNN2D model has advanced performance, attaining the best values. The graphs above visually represent these findings.

6. CONCLUSION:

This work highlights the pressing necessity for an effective and dependable approach to forecast adverse Drug Reactions (ADRs) on account of drug-drug interactions, a giant public health issue. Present day detection processes are often constrained, as they predominantly depend on post-marketing reviews and fail to recognize rare drug interactions prior to a medicine's market advent. To treatment this deficiency, the "sides Drug bank" dataset was hired, offering crucial insights into drug interactions and their corresponding aspect results. The system attained a wonderful overall performance enhancement, with an accuracy of 99.744246%, by utilizing superior machine learning methodologies, in particular 2d Convolutional Neural Networks (CNN). This technique considerably improves ADR detection, offering a feasible answer for the early prediction of unfavourable drug interactions and mitigating related health risks. The superior performance of the CNN model illustrates its ability to revolutionize current ADR detection methodologies, improving patient protection and healthcare results.

The future potential of this system is improving the precision and scalability of ADR detection by means of the integration of larger, more assorted datasets and the investigation of superior methodologies which includes deep reinforcement learning or multi-modal learning. Moreover, the integration of actual-time monitoring of drug interactions with affected person-unique information could facilitate early diagnosis and tailor-made protection advice. Extending the version to embody a much wider array of pharmaceuticals and interactions may decorate its standard relevance and efficacy.

REFERENCES:

[1] Coleman, J. J., & Pontefract, S. K. (2016). Adverse drug reactions. *Clin. Med.*, 16(5), 481-485.

[2] Jiang, H., Lin, Y., Ren, W., Fang, Z., Liu, Y., Tan, X., Lv, X., & Zhang, N. (2011). Adverse drug reactions and correlations with drug–drug interactions: A retrospective study of reports from 2011 to 2020. *Frontiers Pharmacol*, 13(2), 1- 14.

[3] L. Zou, L., X. Luo, X., Y. Zhang, Y., X. Yang, X., & and X. Wang, X. (2023). HC-DTTSVM: A network intrusion detection method based on decision tree twin support vector machine and hierarchical clustering. *IEEE Access*, 11(1), 21404–21416.

[4] Jabeen, T., Ashraf, H., & Ullah, A. (2021). A survey on healthcare data security in wireless body area networks. *J. Ambient Intell. Humanized Comput*., 12(2), 9841–9854.

[5] Angamo, M. T., Chalmers, L., Curtain, C. M., & Bereznicki, L. R. E. (2016). Adverse-Drug-Reaction-Related hospitalisations in developed and developing countries: A review of prevalence and contributing factors. *Drug Saf*., 39(9), 847–857.

[6] Kim, C., & Tatonetti, N. (2021). Prediction of adverse drug reactions associated with drug-drug interactions using hierarchical classification. *bioRxiv*, 2(3), 1-41.

[7] Palleria, C., Di Paolo, A., Giofrè, C., Caglioti, C., Leuzzi, G.., Siniscalchi, A., De Sarro, G., & Gallelli, L. (2013). Pharmacokinetic drug-drug interaction and their implication in clinical management. *J. Res. Med. Sciences*, 18(7), 601-610.

[8] Chen, M., Jiang, Y., Lei, X., Pan, Y., Ji, C., & Jiang, W. (2024). Drug target interactions prediction based on signed heterogeneous graph neural networks. *Chin. J. Electron*., 33(1), 231–244.

[9] Castiglione, F., Nardini, C., Onofri, E., Pedicini, M., & Tieri, P. (2023). Explainable drug repurposing approach from biased random walks. *IEEE/ACM Trans. Comput. Biol. Bioinf.*, 20(2), 1009–1019.

[10] Abbas, S., Avelino Sampedro, G., Abisado, M., Almadhor, A. S., Kim, T. H., & Mohamed Zaidi, M. (2023). A novel drug-drug indicator dataset and ensemble stacking model for detection and classification of drug-drug interaction indicators. *IEEE Access*, 11(2), 101525–101536.

[11] Paltun, B. G., Kaski, S., & Mamitsuka, H. (2022). DIVERSE: Bayesian data Integrati VE learning for precise drug ResponSE prediction. *IEEE/ACM Trans. Comput. Biol. Bioinf*., 19(4), 2197–2207.

[12] He, H., Chen, G., & Yu-Chian Chen, C. (2022). 3DGT-DDI: 3D graph and text based neural network for drug–drug interaction prediction. *Briefings Bioinf.*, 23(3), 1-15.

[13] Deng, Y., Xu, X., Qiu, Y., Xia, J., Zhang, W., & Liu, S. (2020). A multimodal deep learning framework for predicting drug–drug interaction events. *Bioinformatics*, 36(15), 4316–4322.

[14] Abdel-Basset, M., Hawash, H., Elhoseny, M., Chakrabortty, R. K., & Ryan, M. (2020). Deep H-DTA: Deep learning for predicting drug-target interactions: A case study of COVID-19 drug repurposing. *IEEE Access*, 8(2), 170433–170451.

[15] Liu, J., Huang, Z., Ren, F., & Hua, L. (2019). Drug-drug interaction extraction based on transfer weight matrix and memory network. *IEEE Access*, 7(3), 101260–101268.

[16] Karim, M. R., Cochez, M., Jares, J. B., Uddin, M., Beyan, O., & Decker, S. (2019). Drug-drug interaction prediction based on knowledge graph embeddings and convolutional-LSTM network. *in Proc. 10th ACM Int. Conf. Bioinf., Comput. Biol. Health Informat*., 2(1), 113–123.

[17] Liu J., Huang, Z., Ren, F., & Hua, L. (2019). Drug-drug interaction extraction based on transfer weight matrix and memory network. *IEEE Access*, 7(2), 101260–101268.

[18] Bongini, F., Scarselli, M., Bianchini, G. M., Dimitri, N., Pancino, & Lió, P. (2023). Modular multi–source prediction of drug side–effects with DruGNN. *IEEE/ACM Trans. Comput. Biol. Bioinf*., 20(2), 1211–1220.

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