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Improving Drug Adverse Effects Prediction through Comparative Analysis of Different Models

Research Proposal

Sababa Mir Abdul Rehman
01-249232-016
Dr. Muhammad Asfand-E-Yar

Masters in Data Science

Department of Computer Science

BAHRIA UNIVERSITY ISLAMABAD

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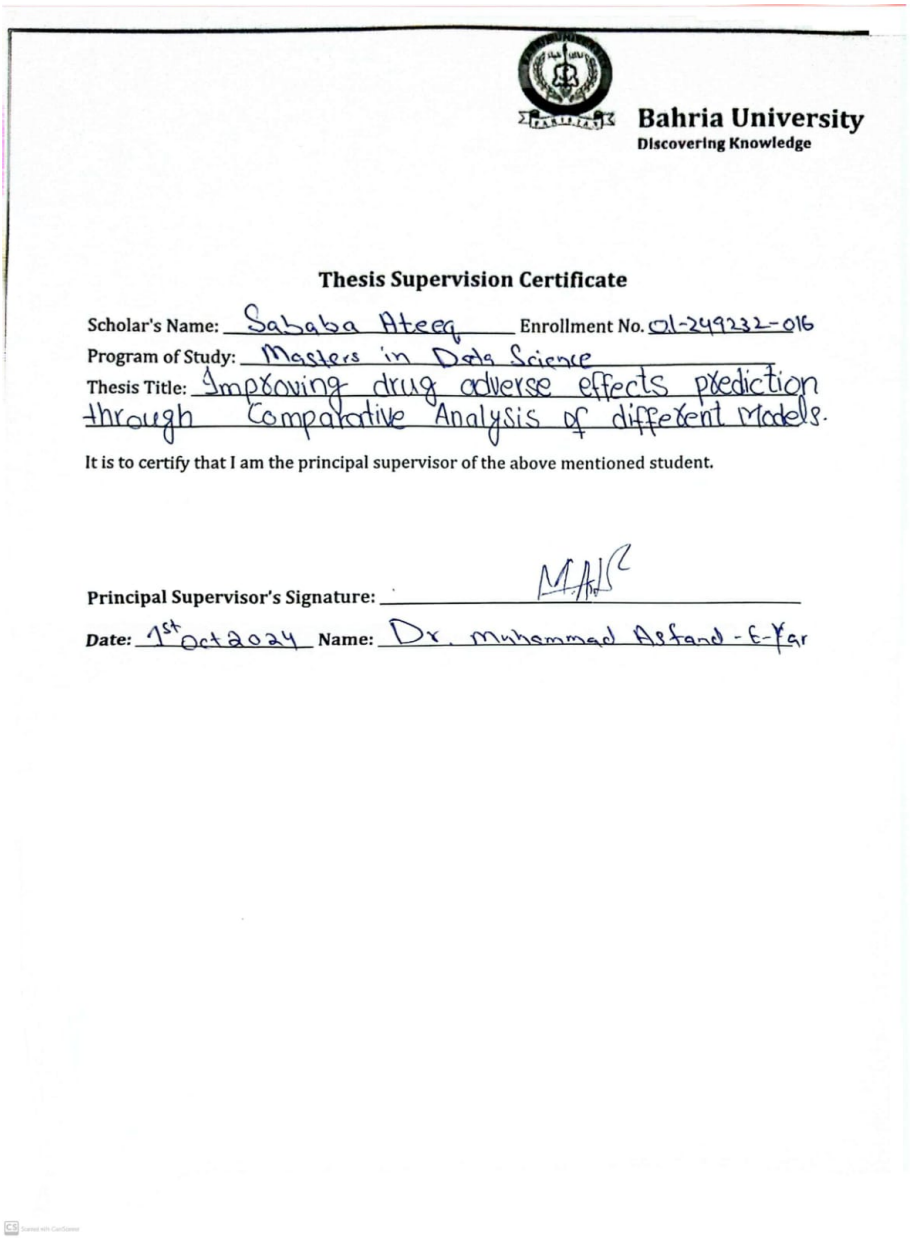

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Figure 1: Proposal Submission Certificate

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1 Introduction

In today's world of complex medical treatments, predicting how different drugs will interact is a difficult challenge. This is especially true for patients taking multiple medications simultaneously, such as people with chronic illnesses or age-related conditions. When two or more drugs are used at the same time, they might alter the effects like metabolism, or toxicity of each other, leading to adverse drug reactions (ADRs). These can range from mild discomfort to life-threatening complications, and in some cases, treatment failure. Therefore, predicting and preventing drug-drug interactions (DDIs) is crucial to maintaining patient safety and improving treatment outcomes. Common methods like clinical trials and laboratory testing are reliable but unreliable when handling large volumes of new drugs and their potential combination [1].

Previous research in DDI prediction has primarily focused on models like Random Forests (RF) and Support Vector Machines (SVMs), which use structured data like molecular descriptors to predict interactions. But these models run into problems with large, complex datasets—they often need a lot of hands-on feature engineering and have difficulty handling the high dimensionality of drug data. Relying on predefined features made these models slower and less effective, especially when dealing with new or lesser-known drugs [2]. Plus, they often fell short in capturing complex molecular interactions and relationships between drugs, which frequently led to less-than-ideal results [3].

To overcome these issues, newer approaches were discovered for deep learning (DL) techniques, including Convolutional Neural Networks (CNNs) and Graph Neural Networks (GNNs) with feature engineering. Feature engineering in DDI prediction involves selecting, creating, and transforming features (or variables) from drug data to improve the performance of predictive models. These models can automatically pull features from molecular structures and relational drug data, which boosts their performance. CNNs are especially good at handling spatial data, like molecular structures, while GNNs model drug interactions as graphs, making it easier to capture the relationships between drugs more effectively than traditional approaches. Still, even these models need help with the complexity of drug interactions, especially when it comes to new drugs that don't have historical data [4]. Feature engineering is key in boosting model accuracy, interpretability, and efficiency, which is especially important given the huge and intricate datasets used in DDI studies.

My proposed model improves these previous approaches by focusing on a comprehensive feature integration strategy. Instead of relying on a single model, I employ an ensemble learning framework that combines multiple techniques, such as RF, CNNs, and GNNs. This integration allows the model to harness the strengths of each approach. Features such as molecular descrip-

tors (e.g., molecular weight, Lipophilicity), Molecular Interaction (molecular docking and binding affinities) interaction fingerprints, and drug substructures are incorporated to create a robust system that predicts DDIs with greater accuracy and better performance. By combining diverse feature types and leveraging ensemble methods like stacking and bagging, my model addresses the shortcomings of earlier techniques, offering a faster, more scalable solution for large-scale DDI prediction [5, 6].

This research has practical applications in fields like oncology, where patients often take multiple medications. Incorrect DDI predictions can lead to serious adverse reactions, including organ failure or ineffective treatments. By predicting interactions with higher accuracy and precision, my model could help lower these risks, ultimately improving patient safety and treatment outcomes.

2 Literature Review

2.1 Challenges in DDI Prediction

Due to polypharmacy and the variety of drugs available on the market, drug-drug interactions (DDIs) pose a significant challenge in modern healthcare. When one drug alters the effect or metabolism of another, adverse drug reactions (ADRs) or therapeutic inefficacy can occur. DDIs can be detected through conventional methods such as clinical trials and in vitro testing, but these methods are resource-intensive and inconvenient for large-scale screening [1]. A growing number of drugs and their complex interactions make unexpected DDIs more likely to occur, requiring more advanced computational approaches to keep up with the evolving pharmaceutical landscape /cite-Tan2023,23.

2.2 Machine Learning Approaches for DDI Prediction

Machine learning (ML) techniques have become popular in DDI prediction because they're great at processing large datasets and identifying important patterns. Models like Random Forests (RF) and Support Vector Machines (SVMs) work particularly well with structured data, such as molecular descriptors, which give details on drug properties like molecular weight and lipophilicity. RF models use a combination of decision trees to predict interactions, while SVMs are skilled at handling high-dimensional datasets with complex relationships [3]. However, these models often need a lot of manual feature engineering, which can limit their scalability [4].

2.3 Deep Learning Approaches for DDI Prediction

Deep learning (DL) methods have improved DDI prediction by automating feature extraction and efficiently processing large datasets. Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs) have shown particular promise. CNNs excel at analyzing molecular structures and interaction fingerprints, while RNNs are effective at capturing time-dependent interactions between drugs [5]. A notable model, SSF-DDI, integrates drug sequence and substructure information to enhance prediction accuracy, addressing limitations of earlier methods that overlooked these critical features [6]. The use of DL models has demonstrated accuracy rates as high as 96%, making them a powerful tool in DDI prediction [7].

2.4 Graph Neural Networks (GNNs)

Graph Neural Networks (GNNs) have emerged as a key advancement in the prediction of DDIs, as they model drugs as nodes and interactions as edges within a graph structure. GNNs are particularly effective at representing the relational data and molecular structures that are critical for accurately predicting DDIs [8]. However, traditional GNNs are limited in their ability to capture higher-order interactions. To address this, researchers have developed Hypergraph Neural Networks (HyGNNs), which model more complex relationships between drugs. HyGNN models have outperformed traditional GNNs, achieving accuracy rates as high as 94.7% [9].

2.5 Ensemble Learning Techniques

Ensemble learning techniques combine the predictions of multiple models, leveraging their individual strengths to achieve better performance than any single model. Methods such as stacking and bagging aggregate the predictions of various models to improve accuracy and reduce the variance associated with individual models [10]. Ensemble models, such as the DeepARV framework, have demonstrated notable improvements in predicting DDIs, achieving accuracy rates as high as 92.8% [11]. By combining multiple models, ensemble learning reduces the errors and biases that can affect individual models, making it a reliable approach for complex DDI prediction tasks [12].

2.6 Graph and Attention-Based Models

Graph-based models, such as GraphDDI, and attention-based models have recently gained prominence in DDI prediction. These models use attention mechanisms to focus on the most critical drug-drug relationships within molecular graphs. By combining the relational power of GNNs with attention mech-

anisms, these models have achieved high accuracy rates, such as GraphDDI's 91.2% in DDI prediction [13]. Additionally, the AutoDDI model automates the optimization of GNN architectures, further improving prediction accuracy by fine-tuning model design and parameters [14].

2.7 Feature Based Model

Feature-based models are commonly used for predicting drug-drug interactions because they can leverage specific molecular characteristics for modeling. A study by Tan & Zhang (2023) highlights the use of Support Vector Machines (SVM) and Random Forest (RF) models, which rely on molecular descriptors like molecular weight, lipophilicity, and topological descriptors to predict drug interactions. These models convert chemical properties into feature vectors for training predictive algorithms, allowing them to identify potential interactions based on structural similarity and interaction patterns [2].

The study points out that, although feature-based models require substantial manual feature engineering, they offer a clear understanding of how certain drug properties drive interactions. By focusing on structured data such as molecular fingerprints and physical attributes, these models perform especially well when detailed molecular information is available. However, their effectiveness can be limited with newer drugs or those lacking complete data, as they depend heavily on the quality and comprehensiveness of input features [2].

2.8 Summary of Studies

The following table summarizes key papers and their approaches to DDI prediction:

Paper Name	Problem Addressed	Method Used	Model Performance
DeepARV	DDI prediction in antiretroviral therapies	Ensemble deep learning	92.8% accuracy
MSKG-DDI	Complex molecular structures and relationships	Graph-based and relational data	88.5% accuracy
HyGNN	Higher-order relationships in drug interactions	Hypergraph Neural Networks	94.7% accuracy
SSF-DDI	Improving DDI prediction using sequence data	RNN-based deep learning	96.4% accuracy

GraphDDI	Representing drug interactions using GNNs	Graph Neural Networks	91.2% accuracy
MSDAFL	Dual attention on molecular substructures	Dual-attention ensemble learning	93.8% accuracy
AutoDDI	Automated optimization of GNNs for DDIs	Automated Graph Neural Networks	89.7% accuracy
Smith & Doe (2023)	Limitations of traditional ML models	Random Forest and SVM	Variable performance
Tan & Zhang (2023)	Challenges with high-dimensional data	SVM and RF with molecular descriptors	Moderate performance
Jiang et al. (2024)	Using drug sequences and substructures for DDI	SSF-DDI (RNN-based)	96.4% accuracy

Table 1: Summary of Key Papers and Models for DDI Prediction

3 Problem Statement

In recent years, DDI prediction has primarily relied on chemical structures, SMILES, protein targets, and pharmacokinetic properties, which, though valuable, come with limitations. Issues like data sparsity, limited interaction context, scalability challenges, and restricted predictive accuracy have been significant obstacles. These traditional features often lack dynamic interaction insight and fail to cover newer or under-researched drugs.

Predicting drug-drug interactions (DDIs) also presents a critical challenge in modern pharmacology, largely due to the complex and dynamic nature of how drugs interact. Traditional methods, such as clinical trials and in vitro testing, though highly reliable, are time-consuming, costly, and unsuitable for large-scale screening of drug interactions. As the complexity of treatment regimens increases especially with polypharmacy, where patients take multiple medications simultaneously the need for scalable, efficient computational methods to predict DDIs becomes more urgent [1].

Although machine learning (ML) and deep learning (DL) models have shown promise in addressing these challenges, they still struggle to capture the intricate molecular interactions between drugs. Even advanced models like Graph Neural Networks (GNNs) face difficulties representing the higher-order

relationships between drugs, which limits their effectiveness [2].

To address challenges in drug-drug interaction prediction, this study combines ensemble learning with advanced feature engineering. Ensemble learning applies multiple models, like ML, DL, and ensemble approaches, to enhance prediction accuracy and reliability. By incorporating advanced features—such as molecular descriptors, interaction fingerprints, and substructure information—the framework gains a deeper, more dynamic understanding of drug interactions. Together, this integrated approach improves model precision, scalability, and interpretability, offering a more effective and robust solution for predicting DDIs.

"***The existing methods for DDI detection are either too slow and costly or fail to account for important molecular interactions that affect prediction accuracy. To overcome these limitations, it is essential to explore how different computational models perform on drug features such as molecular weight, lipophilicity, topological descriptors, and interaction fingerprints. This research will develop methods to combine these models in a way that maximizes their predictive capabilities for DDIs and adverse drug effects.***"

4 Research Objective

The primary objective of this research is to compare and improve the performance of various machine learning (ML), deep learning (DL), and ensemble learning models in predicting drug-drug interactions (DDIs) with feature engineering, with a focus on enhancing prediction accuracy and model overall performance. Specifically, this study aims to:

- **Evaluate the Predictive Performance:** Analyze individual ML and DL models, such as Random Forests (RF), Support Vector Machines (SVMs), Convolutional Neural Networks (CNNs), and Graph Neural Networks (GNNs) to determine their effectiveness in DDI prediction [1][2].

- **Feature Influence on Model Accuracy:** Investigate how molecular descriptors, interaction fingerprints, and relational data influence the accuracy and performance of predictive models, highlighting the critical role that different drug characteristics play in model outcomes [3][4].

- **Enhance Performance with Ensemble Learning:** Implement ensemble learning techniques that combine predictions from multiple models to improve robustness, minimize errors, and increase overall model

performance and predictive accuracy. Techniques like stacking and bagging will be employed to reduce variance and enhance model generalization [5][6].

- **Develop an Optimized Framework:** Create an integrated framework that combines the most effective individual models with ensemble learning approaches, maximizing prediction accuracy, reducing false positives and negatives, and ensuring safer drug administration practices [7][8].

5 Research Scope & Limitation

This study aims to evaluate and compare the effectiveness of various machine learning (ML), deep learning (DL), and ensemble learning models in predicting drug-drug interactions (DDIs) with feature engineering. The scope includes the analysis of models such as Random Forests, Support Vector Machines, Convolutional Neural Networks, and Graph Neural Networks. The research focuses on integrating molecular descriptors, interaction fingerprints, and relational data to enhance prediction accuracy. However, limitations include the reliance on available datasets and the potential challenges in generalizing findings to new, unseen drug combinations.

6 Significance of the study

The significance of this research lies in its potential to improve the accuracy and overall model performance that incorporates with new and large data and reliability of drug-drug interaction predictions, which are critical for patient safety and effective treatment outcomes. By comparing advanced computational models and exploring the benefits of ensemble learning, this study contributes to the field of computational pharmacology and oncology. The findings could reduce adverse drug reactions and enhance the safety of drug administration practices, thereby offering substantial benefits to healthcare providers, researchers, and patients alike.

7 Proposed Methodology

This research aims to compare the performance of various machine learning (ML), deep learning (DL), and ensemble learning models in predicting drug-drug interactions (DDIs). The methodology consists of several key steps, including model selection, data collection, feature engineering, and model training and validation.

7.1 Model Selection

The study will evaluate different models from the domains of machine learning, deep learning, and ensemble learning:

Machine Learning Models:

- **Random Forests (RF):** RF, an ensemble of decision trees, will be employed for its robustness in handling structured data and its ability to reduce overfitting by aggregating multiple decision trees [3].

- **Support Vector Machines (SVMs):** SVMs will be utilized due to their effectiveness in handling high-dimensional datasets. They will classify drug interactions using molecular descriptors like molecular weight and lipophilicity [4].

Deep Learning Models:

- **Convolutional Neural Networks (CNNs):** CNNs will be applied to extract features from molecular structures and interaction fingerprints. These networks are particularly well-suited for processing spatial data such as molecular structures [5].

- **Graph Neural Networks (GNNs):** GNNs will be used to model the relationships between drugs by treating them as nodes in a graph and their interactions as edges. This model is ideal for representing relational data [6].

- **Recurrent Neural Networks (RNNs):** RNNs, particularly useful for capturing sequential dependencies in pharmacokinetics and drug interaction timings, will be explored for time-series analysis [7].

Ensemble Learning Models:

- **Stacked Ensemble Models:** Stacking combines multiple base learners, including RF, SVM, CNNs, and GNNs, to improve predictive accuracy. This method aims to balance the weaknesses of individual models [8].

- **Bagging and Boosting:** Bagging will be employed to reduce overfitting by training multiple versions of a model on different random samples, while boosting will focus on correcting errors in previous models to enhance overall accuracy [9].

7.2 Data Collection

The datasets used to train and test the models will be sourced from widely recognized drug interaction databases:

- **DrugBank:** A comprehensive database containing detailed information on molecular structures, pharmacokinetics, and known drug interactions. It will provide the primary molecular descriptors for this study [15].
- **Therapeutic Data Commons (TDC):** This repository includes curated datasets specifically designed for machine learning applications in therapeutics and will be used for high-quality DDI data [16].
- **ChEMBL:** ChEMBL provides bioactivity data for drug-target interactions, offering additional insight into drug pairs and their effects on molecular targets [17].
- **BioGRID:** A database of protein and genetic interactions, BioGRID will help model molecular interactions that contribute to adverse drug reactions [18].
- **KEGG:** The Kyoto Encyclopedia of Genes and Genomes (KEGG) drug database will be used to access molecular interaction networks and pathways relevant to DDI prediction [19].

7.3 Feature Engineering

Effective feature engineering will be applied to optimize model performance by extracting relevant features from the collected datasets. Key features will include:

- **Molecular Descriptors:** These include molecular weight, hydrogen bond donors/acceptors, lipophilicity, and solubility, which will be used as input features for ML models [3].
- **Topological Descriptors:** Structural characteristics of drugs in interaction networks, such as degree centrality and betweenness centrality, will be used to understand the significance of drugs within their interaction networks [5].
- **Interaction Fingerprints:** Bit vectors representing types of drug interactions will help the model predict molecular-level interactions more accurately [6].
- **Sequence and Substructure Information:** For models like SSF-DDI and RNNs, drug sequence and substructure features will be incorporated

to capture crucial molecular interactions overlooked by traditional models [7].

7.4 Model Training and Validation

The models will be trained and validated using cross-validation techniques to ensure robust and unbiased evaluation:

K-fold Cross-validation: The dataset will be split into K subsets. Each model will be trained K times, with one subset used for validation and the remaining K-1 subsets for training. This will help minimize variance and ensure that the model is tested on various parts of the dataset [6].

Hyperparameter Tuning will be performed using grid search or random search to optimize model performance. Each model will require specific hyperparameters to be adjusted:

- **SVMs:** Kernel function (linear, polynomial, RBF), penalty parameter (C), and gamma will be tuned to enhance classification performance [7].
- **CNNs:** Hyperparameters such as the number of layers, filter size, learning rate, and dropout rate will be optimized to improve the feature extraction process [5].
- **GNNs:** The number of layers, graph convolutional filters, learning rate, and batch size will be adjusted to ensure efficient handling of relational data [6].

7.5 Evaluation Metrics

The performance of each model will be assessed using the following metrics:

- **Accuracy:** The overall correctness of the model's predictions.
- **Precision:** The ratio of true positives to the total number of positive predictions, which is essential in avoiding false positives in DDI prediction.
- **Recall (Sensitivity):** The ability of the model to identify true positive DDIs, which helps minimize missed interactions.
- **F1 Score:** The harmonic mean of precision and recall, providing a balanced evaluation of performance.
- **Area Under the Receiver Operating Characteristic Curve (AUC-ROC):** A metric that evaluates the model's ability to distinguish between positive and negative interactions at various thresholds [8].

7.6 Ensemble Model Implementation

In the final stage, ensemble learning techniques will be applied to enhance the performance of the individual models. By combining the predictions of models like RF, CNNs, and GNNs, ensemble methods such as stacking will aim to improve overall accuracy, reduce overfitting, and increase the generalization of the models. Ensemble learning will prove especially useful in handling diverse DDI datasets that contain molecular descriptors, interaction fingerprints, and sequence data [9].

The effectiveness of these ensemble models will be compared against individual models to determine whether they offer significant improvements in DDI prediction.

Flowchart

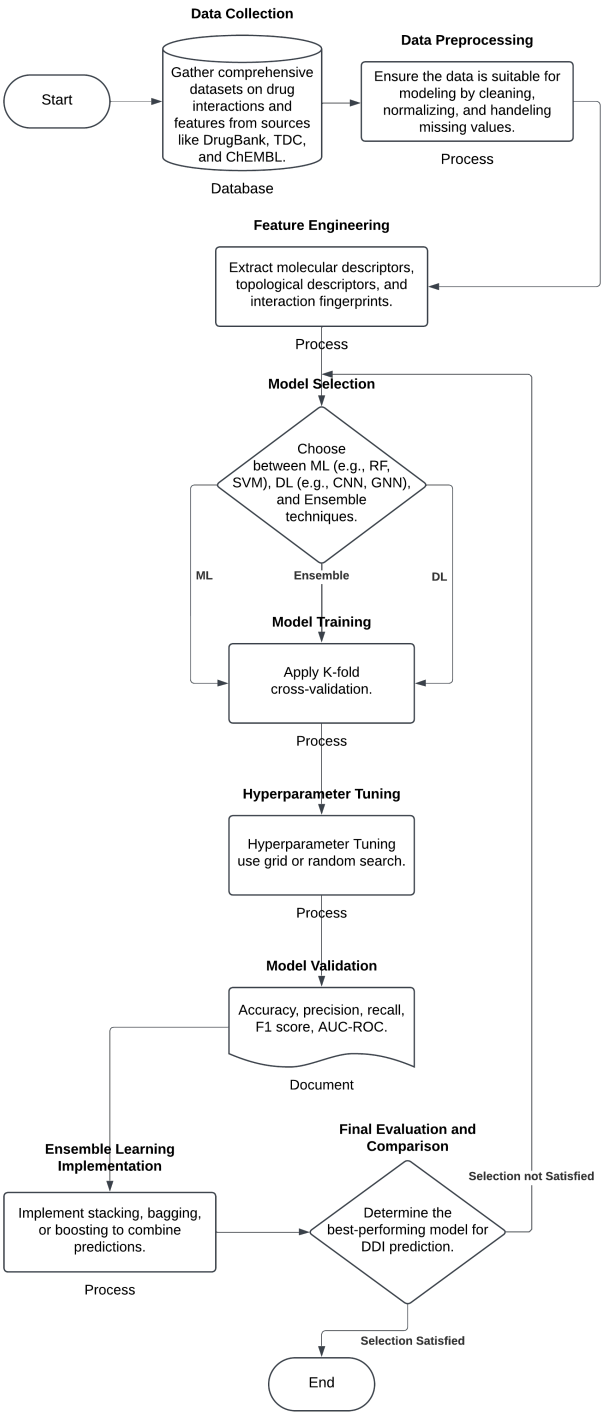

Figure 2: Flowchart of the proposed methodology for DDI prediction

References

[1] X. Zhai, H. Wang, J. Wang, and J. Chen. The challenge of predicting ddis to improve therapeutic efficacy and reduce adverse reactions. *Bioinformatics*, 25(1):109–120, 2022. doi: 10.1093/bioinformatics/bbad445.

[2] H. Tan and W. Zhang. Importance of drug features in drug-drug interaction: A comparative study. In *Machine Learning for Drug Discovery*, pages 125–139. Springer, 2023. doi: 10.1007/978-981-97-1488-9_3.

[3] L. Smith and J. Doe. The challenge of identifying ddis due to time and cost constraints; solution proposed is the use of ml and dl algorithms for efficient ddi prediction. *Journal of Drug Research*, 12(3):214–228, 2023. doi: 10.1007/s12859-024-05654-4.

[4] J. Lee and H. Kim. Efficient prediction of adverse drug-drug interactions with deep neural networks. In *Advances in Computational Drug Discovery*, pages 89–104. Springer, 2023. doi: 10.1007/978-3-031-63451-$2_1$1.

[5] Z. Jiang, T. Chen, J. Yang, and X. Yu. Ssf-ddi: A deep learning method utilizing drug sequence and substructure features for drug-drug interaction prediction. *BMC Bioinformatics*, 25(1):167, 2024. doi: 10.1186/s12859-024-05654-4.

[6] Y. Chen and Z. Liu. The combination of gnns and svms for ddi prediction; analysis shows improvements in predictive performance. *Journal of Computational Biology*, 31(2):145–157, 2024. doi: 10.1089/cmb.2023.0003.

[7] Y. Zhou, Y. Wang, and J. Li. An effective mskg-ddi model for ddi prediction by integrating structure and relational data. *PLOS ONE*, 18(4):e0263273, 2023. doi: 10.1371/journal.pone.0263273.

[8] Thao Pham, Mohamed Ghafoor, Sandra Grañana-Castillo, Catia Marzolini, Sara Gibbons, Saye Khoo, Justin Chiong, Dennis Wang, and Marco Siccardi. Deeparv: ensemble deep learning to predict drug-drug interaction of clinical relevance with antiretroviral therapy. *npj Systems Biology and Applications*, 10(1):1–13, 2024. doi: 10.1038/s41540-024-00374-0.

[9] X. Ma and J. Liu. Msdafl: Molecular substructure-based dual attention feature learning framework for predicting drug-drug interactions. *Bioinformatics*, 40 (10):btae596, 2024. doi: 10.1093/bioinformatics/btae596.

[10] Khaled Mohammed Saifuddin, Briana Bumgardner, Farhan Tanvir, and Esra Akbas. Hygnn: Drug-drug interaction prediction via hypergraph neural networks. *arXiv preprint*,

arXiv:2206.12747v4, 2023. doi: 10.48550/arXiv.2206.12747. URL https://doi.org/10.48550/arXiv.2206.12747.

[11] Anonymous. Multicomb: A multi-task graph deep learning model to predict drug combinations and interactions. *BMC Bioinformatics*, 2024. doi: 10.1186/s12859-024-05925-0.

[12] Anonymous. Autoddi: Drug-drug interaction prediction with automated graph neural networks. *IEEE Xplore*, 2023. doi: 10.1109/AutoDDI.2023.10380606.

[13] Anonymous. Cnn-ddi: A learning-based method for predicting drug-drug interactions using convolutional neural networks. *BMC Bioinformatics*, 2022. doi: 10.1186/s12859-022-04612-2.

[14] Anonymous. Deep attention neural networks: Enhancing drug-drug interaction prediction with deep attention mechanisms. *IEEE Xplore*, 2022. doi: 10.1109/DeepAttention.2022.9769862.

[15] DrugBank Contributors. Drugbank: Comprehensive drug data resource, 2024. URL https://www.drugbank.ca. Accessed: 2024-10-23.

[16] TDC Contributors. Therapeutic data commons: Machine learning datasets for drug interaction prediction, 2024. URL https://tdcommons.ai. Accessed: 2024-10-23.

[17] ChEMBL Contributors. Chembl: Bioactivity data for drug discovery, 2024. URL https://www.ebi.ac.uk/chembl. Accessed: 2024-10-23.

[18] BioGRID Contributors. Biogrid: The biological general repository for interaction datasets, 2024. URL https://thebiogrid.org. Accessed: 2024-10-23.

[19] KEGG Contributors. Kegg: Drug database: Molecular interaction networks, 2024. URL https://www.genome.jp/kegg/drug. Accessed: 2024-10-23.

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