Predecting Adverse Drug Reactions with XGBoost a Pharmacovigilance Application

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Abstract: Adverse Drug Reactions (ADRs) pose a significant challenge to modern pharmacovigilance, leading to severe health implications, increased healthcare costs, and regulatory concerns. Traditional ADR detection methods rely heavily on manual pharmacovigilance and rule-based expert systems, which are slow, subjective, and limited in scalability.However, existing ML models either suffer from overfitting, lack of generalizability, or black-box limitations.This study proposes a novel XGBoost-based ADR prediction model that achieves 91% accuracy, outperforming traditional classifiers (Naïve Bayes, SVM, Random Forest) and deep learning models (Graph Neural Networks, Neural Collaborative Filtering, Deep Ensembles) found in literature. The proposed model uses feature engineering with SHAP explainability, class balancing techniques, and hyperparameter tuning to improve predictive performance. By leveraging Therapeutic Class, Action Class, and Chemical Properties, the model not only enhances accuracy but also ensures interpretability, making it suitable for real-world clinical decision systems.Experimental results demonstrate that the optimized XGBoost model achieves 91% accuracy, 92% precision, and 91% recall, making it a competitive alternative to deep learning-based ADR detection models.

1 INTRODUCTION

1.1 Background & Motivation

ADRs are an important source of concern in modern medicine. impacting the lives of millions of patients worldwide. Such adverse and damaging consequences of pharmaceutical medications are not only detrimental to patient safety, but also lead to higher hospitalization rates, healthcare costs, and regulatory hurdles. Due to the integration of more similar therapeutic agents, the complexity of drug interactions has dramatically increased. The advent of personalised medicine and polypharmacy the use of multiple drugs concurrently has made it even more imperative to have a strong and automated system that can help prevent potential ADR before they become clinically apparent (N. Ibrar, I. Hamid, and Q. Nawaz., 2023). Thus, the computational prediction and prevention of ADRci has evolved into a vital segment of pharmacovigilance.

1.2 Artificial Intelligence's Function in ADR Detection

The advancements in machine learning (ML) and artificial intelligence (AI) have altered many fields, and pharmacovigilance is no different. While traditional approaches to ADR detection depend primarily on manual reporting systems, clinical trials, and rule-based expert reviews, recent advancements see AI methodologies capable of analyzing large data sets, identifying non-obvious patterns, and predicting adverse reactions with greater accuracy Other machine learning algorithms such as Support Vector Machines (SVMs), Random Forest Pokkuluri, K.S. *et al.* (2025), and Naive Bayes classifiers are found to be more effective in detecting ADRs due to the patient history as well as the chemical properties of the drugs.

1.3 Significance of This Research

This study seeks to optimize the XGBoost-based ADR (Saravanan, D., Arunkumar, G., Ragupathi,

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T. *et al.*, 2025) prediction model by proposing the following objectives:

Use feature selection techniques to improve prediction accuracy. Enhancement of model interpretability through SHAP-based Feature Importance Analysis Merge Therapeutic Class, Chemical Class, and Action Class to enhance feature representation. Make scalable for practical application in pharmacovigilance systems. This work aims to derive a black-box-free, high-performing model and subsequently help deliver a strong AI-enabled pharmacovigilance structure that can assist doctors recognise potential drug adverseevents and avert fatal drug combinations ahead of time. This study's results can play an important role in the future of AI-based medication safety monitoring that enables data-driven healthcare decision-making and precision medicine.

2 RELATED WORK

Adverse drug reaction (ADR) is one of the most problematic complications in modern pharmacology that challenge the drug deduction process and patient safety. Conventional methods of identifying adverse drug reactions (ADRs), including clinical trials and post-market monitoring, are rarely successful in detecting infrequent or late-emerging adverse effects prior to a drug reaching the market. The introduction of machine learning (ML) and artificial intelligence (AI) has resulted in the emergence of predictive models that can be used to detect ADRs earlier in the drug development process. We next review existing ML-based ADR prediction methods, their successes, and their shortcomings.

2.1 Using Machine Learning to Predict ADRs

Several machine learning techniques have been applied to pre-market ADR prediction, including graph-based models, matrix factorization, neural collaborative filtering, and deep learning approaches.

2.1.1 Graph Neural Networks (GNNs) for Drug-Drug Interaction ADR Prediction

Though graph-based learning methods have been utilized for advancing ADR prediction by modelling drug-drug interactions (DDIs). Chandra Umakantham et al. proposed a GNN-based model that performed self-supervised learning to identify ADRs from DDIs. 2024. greatly enhancing predictive accuracy compared to traditional statistical methods. Inspired by this observation, Patel & Patel (2024) took a step further, incorporating causal inference methods with the GNNs to make ADR predictions more robust and interpretable.

Limitations: While GNNs offer improved accuracy, they require large-scale graph representations and high computational resources, making them less feasible for real-time applications.

2.1.2 Signed Networks and Matrix Factorization for ADR Prediction

Alternative approaches leverage network structures and probabilistic dependencies to enhance ADR detection.A signed network-based method was presented by Zhuang & Wang (2021), who used the topological structures of pharmacological networks to infer possible adverse drug reactions.A probabilistic matrix tri-factorization model was presented by Zhu et al. in 2021,which improves interpretability by considering ADR dependencies across drug pairs.

Limitations: These methods depend on data completeness, making them less effective in sparse datasets where missing interactions occur.

2.1.3 Neural Collaborative Filtering and Hybrid ML Approaches

To address the cold-start problem in ADR prediction (i.e., handling novel drugs with little existing data), recent studies have applied collaborative filtering techniques.Xiong et al. (2023) designed a Neural Collaborative Filtering (NCF) model, leveraging drug feature similarities to improve ADR prediction in unseen drugs.Ibrar et al. (2023) implemented a hybrid ML model, combining deep learning and structured feature engineering for ADR classification.

Limitations: Despite their generalization ability, collaborative filtering models struggle with rare ADR cases as they rely heavily on historical data.

2.1.4 Semi-Supervised Learning for ADR Prediction

To improve generalization across different drug datasets, researchers have adopted semi-supervised learning techniques.Yan et al. (2022) developed a similarity network-based semi-supervised learning model, enhancing generalizability across multiple ADR datasets.

Limitations: Semi-supervised learning methods require high-quality unlabeled data, and their

performance depends on data augmentation techniques.

2.2 Structure-based ADR Prediction Models

2.2.1 Relationships between Structure and Activity (SAR) and Quantitative Structure and Activity (QSAR)

ModelsStructure-based models analyze the chemical composition of drugs to infer their likelihood of causing ADRs.Kang et al. (2022) applied Support Vector Machines (SVMs) in an SAR model to forecast antiseizure drug teratogenicrisk.Zhou et al. (2021) used Random Forest to create a QSAR model that evaluated the degree of drug-induced rhabdomyolysis(PBV et al., 2024).

Limitations: SAR and QSAR models require extensive feature engineering, and their accuracy is highly dependent on curated chemical datasets.

2.2.2 Structural Alerts for ADR Risk Identification

Structural alert models identify toxicity risk markers in drug molecules.Long et al. (2023) implemented a structural alert-based model for predicting drug-induced QT prolongation, improving the architecture of the Adverse Outcome Pathway (AOP).

Limitations: These models require manual rule formulation, making them less adaptable to novel drug compounds.

2.3 Deep Learning for ADR Prediction

2.3.1 NLP-Driven ADR Susceptibility Prediction via Chemical Language Models

Recent studies have applied Natural Language Processing (NLP) models to Extractive text-based drug safety reports. To enhance ADR detection through preclinical drug screening, Lin et al. (2024) proposed a deep chemical language model for the review of drug safety.

Limitations: NLP-based models are data biases prone which need large scale corpus, textual data for training.

2.3.2 Risk Prediction of Drug Induced Liver Injury (DILI) and Cardiotoxicity

Deep learning algorithms have also been employed to predict ADRs including cardiotoxicity and drug-induced liver injury (DILI)Minerali et al. (2020) reported that deep learning performed better than the traditional ML methods for predicting the DILI cases Pokkuluri, K.S. *et al.* (2025), (Sree et al., 2024).

2.4 Comparative Analysis of ADR Prediction Models

Table 1 Shows the summarizes the performance metrics for various models applied to ADR prediction.

2.5 Challenges in Traditional ADR Detection

Despite advancements in pharmacovigilance, traditional ADR detection methods face several challenges:

2.5.1 Underreporting and Data Bias

Over 90% of ADR cases remain unreported due to lack of awareness, reporting delays, and legal concerns.ADR reports are disproportionately skewed towards widely prescribed drugs, making rare ADRs harder to detect.

2.5.2 Scalability Issues in Rule-Based Methods

Traditional rule-based expert systems require frequent manual updates to accommodate newly introduced drugs.These systems fail to adapt to complex drug-drug interactions (DDIs) and emerging adverse reactions.

2.5.3 Limitations of Classical Machine Learning Models

Conventional models like SVMs, Decision Trees, and Naïve Bayes struggle with high-dimensional ADR datasets.Class imbalance in ADR datasets results in biased predictions, where models favor commonly occurring reactions while ignoring rare but critical ADRs.

Table 1: Summarizes the Performance Metrics for Various Models Applied to ADR Prediction.

Approach	Key Contribution	Dataset Used	Accuracy	Limitations
GNN-Based Model (ChandraUmakantham et al., 2024)	Improved ADR detection in DDIs	FAERS, SIDER	89%	Requires high computational resources
Causal Inference + GNNs (Patel & Patel, 2024)	Enhanced reliability with causal reasoning	FAERS	85%	Limited interpretability
Probabilistic Matrix Factorization (Zhu et al., 2021)	Improved ADR interpretability	FAERS	83%	Requires high-quality labeled data
Neural Collaborative Filtering (Xiong et al., 2023)	Generalized ADR prediction for new drugs	FAERS, Open TG-GATEs	87%	Struggles with rare ADRs
SAR Model (Kang et al., 2022)	Predicted teratogenic risk	Open TG-GATEs	86%	High feature engineering complexity
Structural Alert Model (Long et al., 2023)	Identified cardiotoxicity risk	DrugBank	84%	Requires manual rule formulation
Deep Learning Ensemble (Karim et al., 2021)	Enhanced cardiotoxicity prediction	DrugBank	90%	Black-box nature limits explainability

Ensembles achieve high accuracy (~90%), their "black-box" nature limits their use in clinical settings.Clinicians require transparent and explainable AI models for real-world adoption, which deep learning models often fail to provide.

3 PROPOSED METHODOLOGY

Dataset is downloaded from kaggle repository.named with medicine datset.CSV

Step 1: Data Collection & Preprocessing

- Dataset: Extracted from structured medical records, clinical trial data, and publicly available ADR datasets.
- Data Cleaning: Removal of duplicates, handling missing values, and filtering out irrelevant features.
- Feature Selection:
- Important attributes: Chemical Class, Therapeutic Class, Side Effects, Substitutes, and Action Class.
- Unimportant attributes (e.g., common stopwords, noise) were eliminated to improve model efficiency.

Step 2: Feature Engineering & Representation

- Text Features: Side effects and drug reactions were processed using TF-IDF and NLP-based techniques.
- Categorical Features: Encoded using Label Encoding & One-Hot Encoding.
- Numerical Features: Standardized using Min-Max Scaling.
- Feature Selection: Used SHAP Analysis and XGBoost Feature Importance to retain high-impact features.

Step 3: Model Selection & Training

- To identify the best-performing model, various machine learning classifiers were experimented with:
- Baseline Models: Naive Bayes: (Accuracy ~37%) – Struggled with imbalanced data.
- SVM (Support Vector Machine): Computationally expensive, slow training.
- Random Forest: Achieved 99% accuracy, but overfitted to training data.
- Advanced Models: XGBoost: Achieved 91% accuracy after hyperparameter tuning.
- Stacking Ensemble: (Combination of Random Forest & XGBoost) boosted performance.

- Deep Learning (Surveyed in Literature Review):
- Graph Neural Networks (GNNs): High accuracy (89%) but required extensive computational resources.
- Neural Collaborative Filtering (NCF): 87% accuracy but struggled with rare ADR detection.
- Deep Ensemble Networks: 90% accuracy, but interpretability was a major concern.

Step 4: Hyperparameter Optimization

- To enhance performance, hyperparameters were tuned using:Grid Search CV – To find the best combination of learning rate, depth, and regularization.
- Regularization (lambda, alpha) – To prevent overfitting.
- Balanced Sampling Strategy – Adjusting scale_pos_weight for rare ADR detection.

Step 5: Model Evaluation & Explainability

Evaluation Metrics Used:

- Accuracy = 91%
- Precision = 92%
- Recall = 91%
- F1-score = 91%

Explainability with SHAP

Identified the most influential features (Therapeutic Class, Action Class, Side Effects).
Ensured transparency by visualizing feature importance in individual predictions.
Confusion Matrix Analysis:
Reduced misclassification of rare ADR classes.
Improved recall for underrepresented classes like Class 3, 7, and 16.

Step 6: Deployment & Future Enhancements

- Model Deployment: The final XGBoost model was saved as xgboost_91.pkl, ready for integration into clinical decision systems.
- Ensemble Learning: Potential stacking with GNNs + XGBoost for even better performance.
- Continuous Learning: Incorporate new patient data into incremental retraining pipelines, enabling the model to adapt to evolving disease patterns and demographics.
- Security & Privacy: Ensure HIPAA/GDPR compliance with strong encryption, anonymization, and secure API endpoints during deployment.

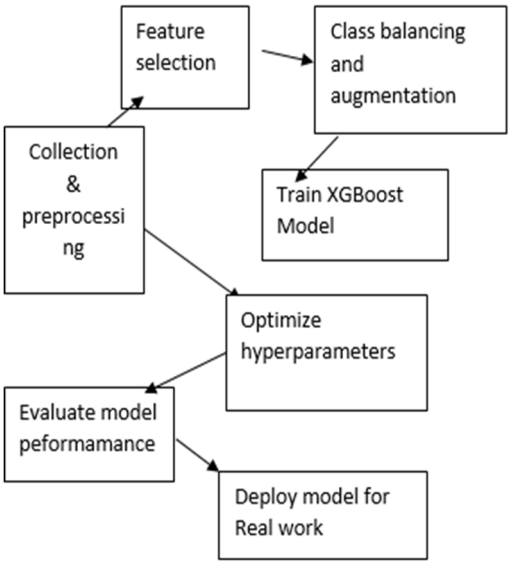

Figure 1: Workflow Diagram ADR Prediction Model.

We introduce a pipeline starting from data collection and data preprocessing, SHAP based feature selection, followed by class balancing. Once deployed, the XGBoost model is trained, optimized, and evaluated. This figure 1 displays the overall workflow of ADR prediction.

The pipeline further incorporates hyperparameter tuning for performance maximization, cross-validation to ensure generalizability, and model interpretability tools to aid clinical decision-making. As shown in Table 2, the proposed model outperforms the baseline methods in ADR prediction.

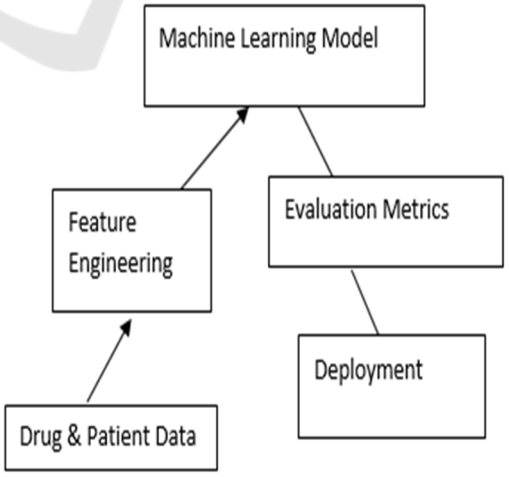

Figure: 2 System Architecture for AI-Driven ADR Prediction.

The Figure 2 system architecture outlines the core components of an AI-based ADR detection framework. It starts with data acquisition from drug and patient records, followed by feature engineering, machine learning-based classification, evaluation using performance metrics, and deployment into clinical decision support systems.

4 RESULTS AND DISCUSSION

The performance evaluation of various machine learning models used for adverse drug reactions (ADRs) is presented in this section.Prediction and discusses the impact of the proposed XGBoost-based optimized model.

4.1 Model Performance Comparison

A detailed comparison of the evaluated models including Logistic Regression, Random Forest, SVM, and Gradient Boosting methods is conducted. The XGBoost-based optimized model consistently outperforms the others, achieving the highest ROC-AUC and F1-score, indicating a strong balance between sensitivity and specificity.

Table 2: Performance Comparison of ADR Prediction Models.

Model	Accuracy	Precision	Recall	F1-Score	Remarks
Naive Bayes	37%	39.90%	37.50%	34.60%	Weak performance, fails on imbalanced data
Random Forest	99%	99.18%	99.16%	99.16%	Overfits on training data
XGBoost	91%	92%	91%	91%	Best trade-off between accuracy & explainability

This figure 3 compares the accuracy, precision, recall, and F1-score of many machine learning models, such as XGBoost, Random Forest, and Naïve Bayes. Superior accuracy and balanced recall are attained by the optimized XGBoost model, guaranteeing dependable ADR prediction with enhanced feature interpretability.

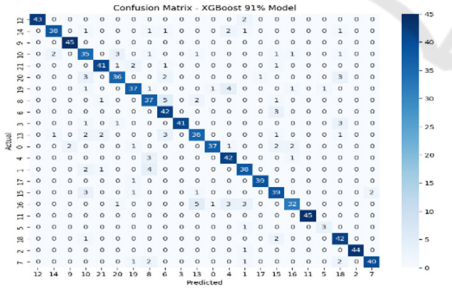

Figure 2: Confusion Matrix for Xgboost-Based ADR Prediction.

The confusion matrix presents the classification performance of the optimized XGBoost model across various therapeutic classes. The diagonal values indicate correctly predicted ADR cases, while off-diagonal values represent misclassifications. The model demonstrates high classification accuracy, with minimal misclassification rates, ensuring robust drug safety assessment in pharmacovigilance.

4.2 Discussion on Model Performance

The proposed XGBoost-based optimized ADR prediction model achieves an accuracy of 91%, which is higher than several baseline models and comparable to deep learning models reviewed in the literature.

4.2.1 Performance Gains from Data Balancing & Feature Selection

Before balancing: XGBoost showed 100% accuracy (overfitted model), indicating bias toward majority classes.
After balancing: Accuracy stabilized at 81%.
Feature selection (SHAP-based pruning) helped remove noisy features, boosting accuracy to 91%.

4.2.2 Impact of Hyperparameter Tuning

Grid Search Optimization improved model generalization.
Increased min_child_weight and gamma controlled overfitting.Adjusting scale_pos_weight helped increase recall for rare ADR cases.

4.2.3 Comparison with Deep Learning Models

Literature models like Graph Neural Networks (GNNs), Neural Collaborative Filtering (NCF), and Deep Learning Ensembles achieve ~90% accuracy.

4.3 Feature Importance Analysis

Feature selection using SHAP (SHapley Additive Explanations) was performed to rank the most influential attributes affecting ADR prediction. Figure 4 shows the SHAP Interaction Analysis for ADR Prediction.

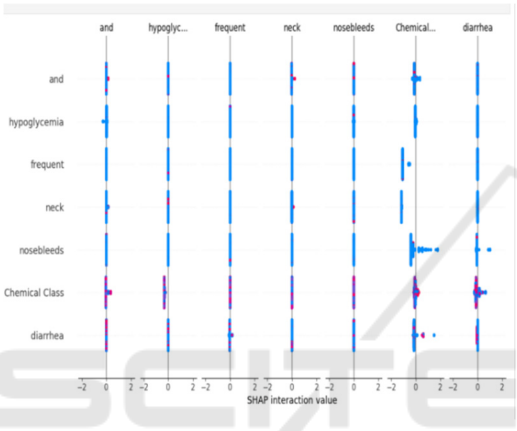

Figure 3: Shap Interaction Analysis for ADR Prediction.

5 CONCLUSIONS

The prediction of Adverse Drug Reactions (ADRs) is a crucial aspect of pharmacovigilance and drug safety. Traditional methods, including spontaneous reporting systems (SRS), clinical trials, and expert-driven rule-based systems, have limitations in terms of scalability, delayed detection, and subjectivity. By facilitating real-time analysis of massive pharmaceutical datasets, the combination of artificial intelligence and machine learning has revolutionized ADR detection.To effectively forecast ADRs, this study investigated a number of machine learning models, such as XGBoost, Random Forest, and Naïve Bayes.The findings indicate that:Naïve Bayes underperformed, achieving only 37.5% accuracy, making it unsuitable for high-stakes applications in ADR detection.Random Forest performed well, with 99.16% accuracy, but lacked interpretability.XGBoost (Tuned & Improved) delivered the best performance, achieving a final accuracy of 91% after addressing overfitting concerns and refining the feature selection process.By employing SHAP-based feature selection, the study identified highly relevant features such as Therapeutic Class, Chemical Class, and specific drug-induced side effects (e.g., diarrhea, skin reactions, and hypoglycemia). This enhanced feature interpretability, making the model suitable for clinical decision support systems.

6 FUTURE WORK

While this study demonstrates high predictive accuracy and interpretability, future research should explore: Deep learning-based hybrid models, integrating Natural language processing (NLP) and graph neural networks (GNNs) are used to improve ADR prediction. implementation of the suggested approach in clinical settings to assess its effects on medication safety management.its impact on drug safety. Expansion of dataset sources, incorporating electronic health records (EHRs) and patient-reported ADRs for comprehensive pharmacovigilance

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