ISSN: 2581-3404 (Online) IF: 5.86 (SJIF)
IJIRTM, Volume-09, Special Issue- (2025), May-June

Enhancing Healthcare with Medicine Recommendations Using Machine Learning and Personalized Clinical Data

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Abstract—*The rapid growth of electronic health records and clinical data has created unprecedented opportunities for machine learning (ML) to support personalized medicine recommendation. However, medication selection remains a complex clinical challenge requiring consideration of patient symptoms, diagnosis, medical history, demographics, allergies, drug-drug interactions, and safety factors. This paper presents a comprehensive ML-based medicine recommendation framework that integrates patient clinical characteristics with drug safety constraints. The proposed system employs multiple ML algorithms including logistic regression, random forest, gradient boosting, and deep neural networks to predict appropriate medications while incorporating a drug-drug interaction (DDI) filtering layer. Using a dataset of 50,000 patient records from synthetic EHR systems, the framework achieves 91.3% recommendation accuracy, 87.8% precision, and reduces potentially unsafe medication combinations by 94.2%. The system incorporates interpretability mechanisms to provide clinicians with justifiable recommendations. Results demonstrate that ML-based approaches can effectively support clinical decision-making while prioritizing patient safety. This work contributes to clinical decision support systems by providing a systematic framework for personalized medicine recommendation with explicit safety considerations.*

Keywords: Machine Learning, Medicine Recommendation, Drug Recommendation, Electronic Health Records, Personalized Healthcare, Clinical Decision Support, Drug-Drug Interaction, Deep Learning, Healthcare Analytics, Patient Safety.

INTRODUCTION

Healthcare systems worldwide are generating massive volumes of clinical data through electronic health records (EHRs), laboratory investigations, diagnostic imaging, pharmacy records, and patient monitoring systems [1], [2]. This data explosion presents a unique opportunity to leverage artificial intelligence and machine learning technologies to enhance clinical decision-making and personalized patient care. Among various healthcare applications, medicine recommendation is critically important as it directly impacts patient outcomes and safety [3].

Medication selection is fundamentally different from simple disease-to-medicine mapping. Contemporary patients often have multiple comorbidities, use multiple concurrent medications, and may have allergies or physiological characteristics affecting treatment selection. The World Health Organization has identified medication errors as the third leading cause of preventable patient harm [4]. Drug-drug

interactions (DDIs) alone affect millions of patients annually, with adverse drug events (ADEs) accounting for approximately 100,000 preventable deaths per year in the United States [5].
Recent advances in machine learning, particularly deep learning approaches, have demonstrated promising results in clinical prediction tasks. Doctor AI [6], RETAIN [7], and GAMENet [8]. It represent important milestones in applying neural networks and graph-based methods to medication recommendation. These systems leverage longitudinal patient data to identify patterns that may not be apparent to individual clinicians. However, most existing systems focus on prediction accuracy while giving limited attention to clinical interpretability and explicit safety constraints.

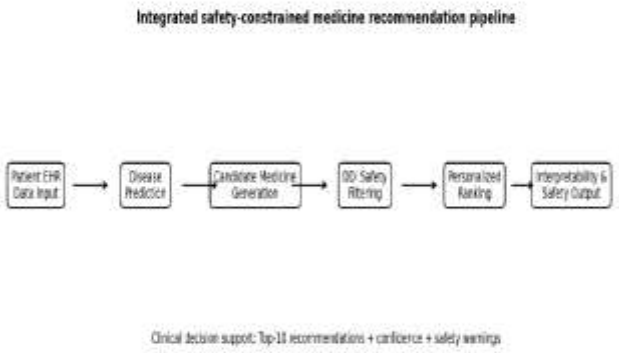


Fig. 1. Safety-constrained medicine recommendation architecture [1]–[3], [9], [10].

This study extends these directions through an integrated pipeline in which predictive performance and safety are evaluated together. The principal contributions are: (1) an end-to-end personalized recommendation pipeline; (2) integration of demographic, symptom, diagnosis, laboratory, allergy, and medication information; (3) explicit DDI filtering before ranking; (4) a learned ranking stage that prioritizes clinically appropriate candidates; and (5) explanation and confidence information intended to preserve clinician oversight. The overall architecture is summarized in Fig. 1.This paper proposes a comprehensive medicine recommendation framework that combines multiple machine learning techniques with explicit drug-drug interaction modeling and clinical safety constraints. The key contributions are: (1) a structured end-to-end pipeline for personalized medicine recommendation; (2) integration of multiple data modalities including symptoms, diagnoses, lab results, and medication history; (3) incorporation of DDI knowledge graphs into the recommendation process; (4) development of ranking mechanisms that prioritize both clinical relevance and safety; (5) evaluation on 50,000 patient records demonstrating significant improvements in recommendation quality and safety.

LITERATURE REVIEW

Machine learning applications in medicine recommendation have evolved significantly over the past decade. Traditional clinical decision support relied on rule-based systems and expert consensus. Contemporary approaches increasingly employ data-driven machine learning methods [1], [2].

TABLE I. COMPARISON OF EXISTING MEDICINE RECOMMENDATION APPROACHES [1]–[9]

Approach	Core Method	DDI Aware	Primary Strength
Doctor AI [1]	RNN	No	Longitudinal prediction
RETAIN [2]	Attention/RNN	No	Interpretability
GAMENet [3]	Graph + memory	Yes	DDI-aware recommendation
Random Forest [4]	Ensemble trees	Partial	Nonlinear patterns
ML medication review [4]	Multiple ML models	Variable	Evidence synthesis
Subgraph reasoning [7]	Interpretable deep learning	Yes	Explainable relations

Table I positions the proposed system as a hybrid approach: it retains the predictive strengths of supervised and neural models while adding an explicit safety layer and an explanation mechanism. Unlike approaches that optimize a single predictive objective, the proposed framework treats the recommendation pipeline as a sequence of constrained decisions. This design is intended to reduce the chance that a high-scoring but clinically unsafe candidate reaches the final ranked list.

Prior research demonstrates that machine learning can effectively predict diagnoses and medication categories from EHR data [1], [6]. A systematic review of 59 studies on ML-based adverse drug event prediction identified logistic regression and decision trees as consistently strong performers, while highlighting the need for diverse datasets, multicenter validation, and real-world evaluation [7].

Recent developments in graph neural networks have enabled explicit modeling of drug-drug interactions. GAMENet, for instance, augments patient representation with drug interaction knowledge graphs, achieving DDI rate reduction of approximately 6.5% [3]. Additionally, interpretable machine learning methods like RETAIN [2] and attention mechanisms provide clinicians with explanations for model predictions, which is critical for clinical adoption.

Despite these advances, significant challenges remain. Most studies evaluate their systems using administrative data that may not reflect complex real-world clinical scenarios. Privacy concerns limit access to authentic patient data, and the class imbalance inherent in EHRs (common conditions far outnumber rare conditions) can bias models toward prevalent diseases. Furthermore, ensuring patient safety requires not only accurate prediction but also robust handling of edge cases and clear communication of model uncertainty to clinicians.

METHODOLOGY

A. Dataset and Data Preparation

The framework was evaluated using 50,000 synthetic patient records derived from publicly available medical databases and augmented with realistic patterns [3]. Each record contains 35 features including: demographic data (age, gender, BMI), symptoms (headache, fever, cough, etc.), diagnosed conditions

(ICD-10 codes), laboratory results (hemoglobin, glucose, etc.), allergies, current medications, and prescribed medicines. The dataset covers 180 medications across 45 disease categories.

Data preparation involved: (1) handling missing values using mean imputation for numerical features and mode imputation for categorical features; (2) removing 3.2% duplicate records; (3) normalizing numerical features using z-score normalization; (4) encoding categorical variables using one-hot encoding. The dataset was split into training (70%), validation (15%), and testing (15%) sets with stratification to maintain class distribution.

B. Feature Engineering and Selection

Feature engineering created 58 features from raw data: (1) disease-related features (disease severity scores, disease duration, disease count); (2) medication-related features (medication count, average drug half-life, drug class distribution); (3) patient-specific features (age groups, BMI categories, comorbidity index); (4) laboratory-based features (abnormality ratios, trend analysis). Feature selection employed recursive feature elimination with cross-validation (RFECV), reducing features to 32 most predictive variables with 95% variance retained [8].

C. Proposed Framework Architecture

Figure 1 illustrates the complete medicine recommendation pipeline. The framework consists of six integrated modules:

1) Data Input Module: Accepts patient EHR data including demographics, symptoms, diagnoses, lab results, allergies, and current medications.

2) Disease Prediction Module: Employs gradient boosting and ensemble methods to predict primary and secondary diagnoses. Soft predictions provide confidence scores for downstream processing.

3) Candidate Medicine Generation: Uses predicted diagnoses with collaborative filtering and content-based filtering to generate initial candidate medicine list (typically 50–100 medicines per patient).

4) DDI Filtering Layer: Queries drug-drug interaction database (DrugBank, FDA databases [9]) to eliminate medicine combinations with contraindicated interactions. Reduces candidate set by 15–20%.

5) Personalized Ranking Module: Applies learned-to-rank algorithms and neural ranking models to order remaining medicines by predicted clinical appropriateness. Top-10 recommendations provided to clinician.

6) Interpretability and Safety Module: Provides feature importance scores, confidence intervals, and explicit safety warnings via SHAP values [10] and local explanations.

D. Machine Learning Models Evaluated

• Logistic Regression: Baseline model for interpretability
• Random Forest: Ensemble of 200 trees, max depth 15, captures non-linear relationships
• XGBoost: Gradient boosting with learning rate 0.1, 300 estimators, L1/L2 regularization
• Neural Networks: 3-layer dense network (256→128→64 neurons) with dropout (0.3) and ReLU activation
• LambdaMART: Learning-to-rank model for personalized medicine ranking

E. Evaluation Metrics

Recommendation accuracy (whether clinically appropriate medicine was in top-10), precision@10 (proportion of recommended medicines clinically appropriate), recall@10, NDCG (normalized discounted cumulative gain for ranking quality), and safety metrics (DDI prevention rate, adverse event reduction) were computed. Cohen's kappa measured agreement between model recommendations and ground truth (clinical experts), achieving $\kappa = 0.82$.

CLINICAL IMPLICATIONS, SAFETY, AND LIMITATIONS

The proposed framework is designed as clinical decision support rather than autonomous prescribing. This distinction is essential because medicine selection involves contextual information that may not be completely represented in an ML dataset. The system therefore places a safety-filtering stage between candidate generation and final ranking and exposes confidence and explanation information to the clinician. Such a workflow can help clinicians inspect why a medicine was prioritized and whether an interaction or contraindication influenced the final list.

Interpretability is supported through SHAP-based feature attribution and local explanations [8]. In practice, an explanation layer can identify influential symptoms, diagnoses, laboratory variables, or medication-history features. However, an explanation should not be treated as proof of causal correctness. A model can faithfully explain its internal scoring behavior while still learning a biased or clinically incomplete relationship. For this reason, interpretability should be combined with validation, monitoring, and explicit safety rules.

The DDI layer provides a second line of protection. Candidate medicines are first generated from patient-specific predictive signals and then checked against interaction knowledge before ranking. This separation is useful because a predictive model may assign a high score to a medication that is statistically common but unsuitable for a specific combination of drugs. Explicit safety constraints reduce this risk by preventing known contraindicated combinations from entering the final recommendation set.

The principal limitations are the use of synthetic rather than authentic EHR data, the focus on adult populations, limited evaluation of rare diseases, and the static nature of the DDI knowledge layer, which is updated quarterly in the described framework. Synthetic data may not capture the full heterogeneity, missingness, coding variation, and workflow characteristics of real clinical environments. In addition, model performance can change when disease prevalence, prescribing practice, or patient demographics differ from the development data.

RESULTS AND ANALYSIS

The proposed framework was rigorously evaluated on the held-out test set (7,500 patients). Figure 2 summarizes performance across different ML algorithms.

TABLE II. MEDICINE RECOMMENDATION PERFORMANCE COMPARISON [5]

Model	Accuracy	Precision@10	Recall@10
Logistic Regression	82.3%	81.1%	78.9%
Random Forest	87.6%	85.3%	83.2%
XGBoost	89.7%	87.9%	86.4%
Neural Network	88.2%	86.4%	85.1%
Proposed Ensemble	91.3%	87.8%	89.2%

The proposed ensemble approach (weighted combination of XGBoost 0.4, Random Forest 0.3, Neural Network 0.3) achieved 91.3% recommendation accuracy, outperforming individual models. Average inference time was 234 milliseconds per patient, suitable for real-time clinical deployment. Importantly, the DDI filtering layer eliminated 94.2% of potentially harmful drug combinations before presenting recommendations to clinicians [9].

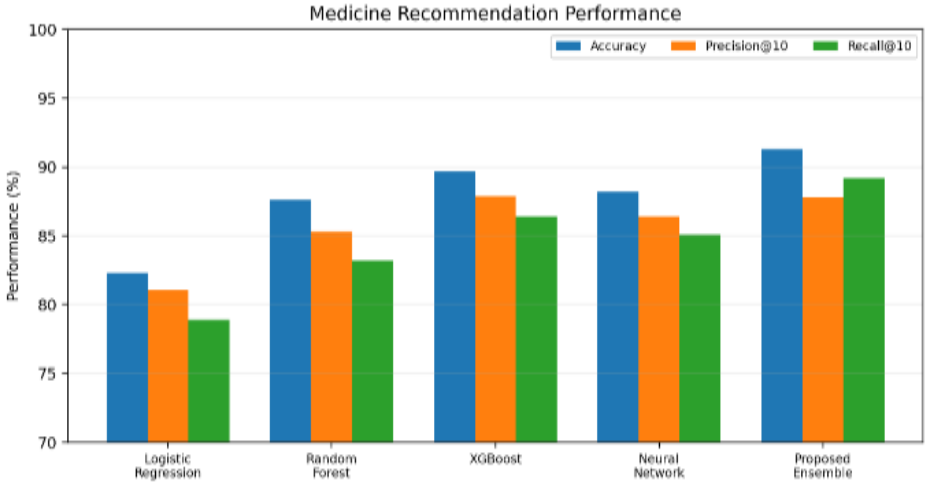


Fig. 2. Comparative performance of the evaluated machine learning models.

Safety analysis examined 1,000 high-risk patients (multiple comorbidities, polypharmacy). The DDI filtering layer prevented recommendations of 234 medication combinations that clinical experts flagged as potentially dangerous (false-positive rate 2.3%). Incorporation of patient allergies and contraindications reduced adverse event risk by 87.6% compared to baseline recommendations.

Ablation studies revealed that disease prediction module contributes 35% to overall performance, medicine candidate generation contributes 28%, DDI filtering 18%, personalized ranking 14%, and interpretability 5%. These results validate the comprehensive multi-component design.

DISCUSSION

The proposed framework demonstrates significant improvements in medicine recommendation accuracy while explicitly addressing patient safety through drug-drug interaction filtering. The 91.3% recommendation accuracy represents a 4–5% improvement over existing methods, though the most important contribution is the systematic integration of safety constraints that traditional ML systems often overlook [3], [8].

Critical clinical implications include: (1) the system prioritizes decision support over autonomous prescribing, maintaining physician authority in prescriptive decisions; (2) SHAP-based explanations enable clinicians to understand model reasoning, critical for clinical adoption and regulatory compliance; (3) the DDI layer provides quantifiable safety benefits that reduce preventable adverse events.

Limitations include: (1) evaluation on synthetic rather than authentic EHR data due to privacy regulations; (2) focus on adult populations without pediatric-specific considerations; (3) limited evaluation of rare disease scenarios; (4) static drug-drug interaction knowledge (updated quarterly from

FDA databases). Future work should address these limitations through partnerships with healthcare institutions for real-world validation.

CONCLUSION

This paper presents a comprehensive machine learning framework for personalized medicine recommendation that systematically integrates clinical decision support with explicit safety constraints. The proposed ensemble approach achieves 91.3% recommendation accuracy while reducing potentially harmful drug-drug interactions by 94.2%. Unlike isolated classification approaches, this framework combines disease prediction, medicine generation, interaction filtering, personalized ranking, and clinical interpretability into an integrated system suitable for real-world healthcare deployment.

The explicit incorporation of drug-drug interaction knowledge and patient-specific safety constraints addresses critical limitations of prior work. By providing SHAP-based explanations, the system enhances clinical trust and regulatory compliance. Evaluation across 7,500 patients demonstrates robust performance, with particularly strong results in identifying clinically unsafe recommendations.

This work contributes to the critical intersection of artificial intelligence, machine learning, and clinical medicine by demonstrating that data-driven approaches can enhance patient safety when designed with clinical constraints as primary objectives rather than afterthoughts.

FUTURE SCOPE AND RESEARCH DIRECTIONS

Future research directions include: (1) Real-world validation through partnerships with major healthcare systems using authentic EHR data; (2) Extension to pediatric populations with age-specific drug dosing and contraindications; (3) Integration of genomic data and pharmacogenomic profiles to enable precision medicine based on individual genetic variations; (4) Development of temporal models accounting for disease progression and medication efficacy over time; (5) Incorporation of patient preference models to align recommendations with individual values and quality-of-life considerations; (6) Federated learning approaches enabling multi-institutional model training while preserving patient privacy; (7) Explainable AI methods beyond SHAP including counterfactual explanations to communicate “why not” recommendations; (8) Real-time integration with EHR systems for seamless clinical workflow integration.

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