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Optimizing Prescription Practices Using AI-Powered Drug Substitution Models to Reduce Unnecessary Healthcare Expenditures in Outpatient Settings

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Abstract

Rising outpatient healthcare costs, particularly due to brand-name and non-optimized drug prescriptions, have created an urgent need for intelligent, cost-saving interventions. Traditional prescribing often overlooks equally effective, lower-cost drug alternatives, leading to significant financial inefficiencies without improving patient outcomes. This study proposes an AI-powered drug substitution model designed to optimize outpatient prescription practices by recommending clinically equivalent and more cost-effective alternatives. The primary goal is to reduce unnecessary healthcare expenditures while preserving treatment quality and physician autonomy. We developed a machine learning-based recommendation system using a comprehensive dataset that includes electronic health records, pharmacy claims, drug equivalency databases, and insurance formulary information. The model was trained to identify optimal drug substitutions based on diagnosis, prescription history, cost, and insurance coverage. Evaluation metrics included substitution precision, potential cost savings, and physician usability testing.

Keywords

Healthcare, Machine Learning, Electronic Health

1. Introduction

1.1. Background

The rising cost of healthcare has become a pressing issue globally, with pharmaceutical spending being one of the most rapidly increasing components. In outpatient care settings, prescription medications constitute a major part of overall medical expenses. This is particularly significant in the treatment of chronic diseases, such as hypertension, diabetes, and hyperlipidemia, where long-term medication use is essential. While innovations in drug development have provided a wider range of therapeutic options, they have also led to the widespread use of expensive brand-name drugs—even in cases where equally effective and more affordable generics or therapeutic alternatives exist. According to the IMS Institute for Healthcare Informatics, nearly $200 billion could be saved annually in the United States alone by optimizing the use of generic drugs and reducing therapeutic duplication [1].

Despite ongoing reforms and policy efforts aimed at promoting rational drug use, a large number of prescriptions continue to be written without proper consideration of available cost-saving alternatives. This is especially true in outpatient settings, where physicians face tight schedules, information overload, and limited decision support during prescribing. Moreover, real-time cost visibility, insurance coverage data, and evidence-based substitution guidance are often absent at the point of care [2]. As a result, prescribing decisions may default to familiar, branded, or previously used drugs, perpetuating inefficiencies and avoidable healthcare expenditure. The disconnection between clinical decision-making and economic consideration underscores the need for an intelligent, scalable, and clinically informed solution.

These challenges—ranging from data breaches and supply chain disruptions to workforce shortages and clinical trial issues—can be mitigated through AI-driven solutions, as summarized in **Figure 1**.

1.2. Justification for the Study

In an era where data-driven decision-making is reshaping industries, healthcare systems are increasingly looking to artificial intelligence (AI) to enhance efficiency, accuracy, and cost control. While AI has made significant inroads into diagnostic imaging, personalized medicine, and operational workflows, its application in drug substitution remains underdeveloped. Most existing tools for drug substitution rely on static drug formularies or simplistic cost comparisons, lacking the contextual intelligence necessary for nuanced prescription decisions. Furthermore, existing e-prescription platforms are typically reactive—alerting providers only when a drug is unavailable or contraindicated—rather than proactively recommending clinically equivalent, lower-cost alternatives.

To bridge this gap, the present study explores the development and implementation of an AI-powered drug substitution model tailored to outpatient clinical workflows. By harnessing machine learning algorithms trained on real-world

data—including prescription histories, patient demographics, cost information, and clinical guidelines, this model aims to provide real-time, personalized substitution suggestions that optimize both therapeutic outcomes and cost efficiency. This approach not only supports physicians in delivering high-quality care but also aligns with the broader objectives of value-based healthcare systems that seek to reduce waste and improve affordability [4] [5].

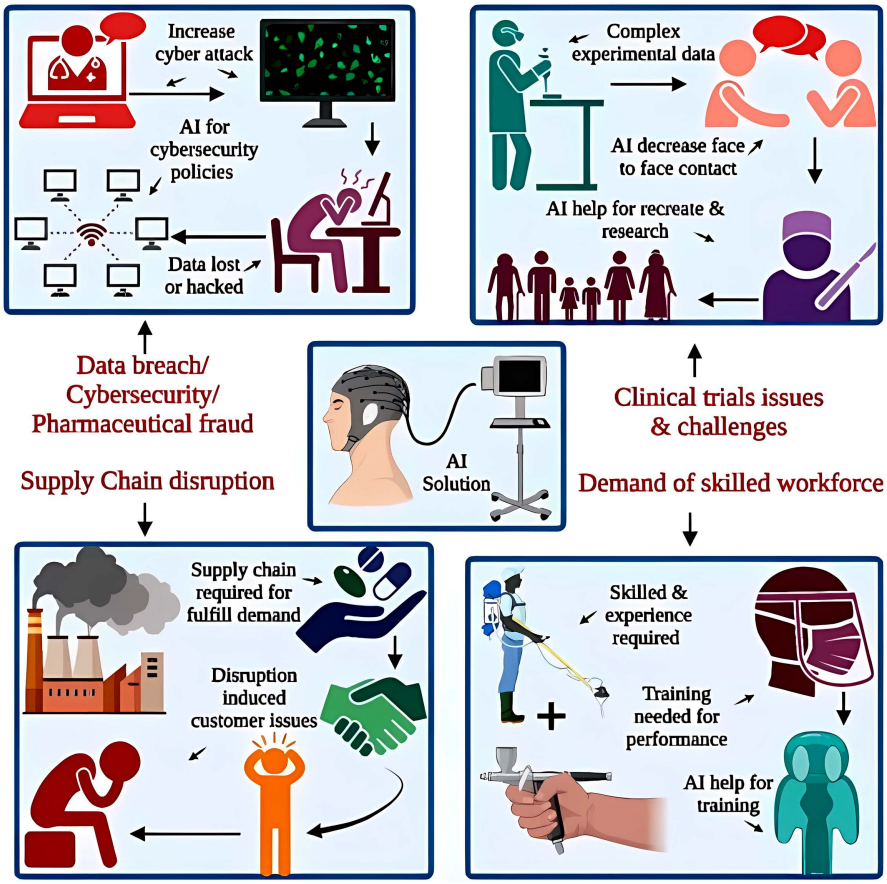

Figure 1. Challenges and AI solutions in pharmaceutical R&D [3].

1.3. Research Goal

The overarching goal of this study is to design, train, and evaluate an AI-based decision support tool capable of recommending lower-cost, clinically appropriate drug alternatives during the prescribing process in outpatient settings. The model aims to combine clinical relevance, economic impact, and workflow compatibility, ensuring it can be seamlessly adopted by healthcare professionals without increasing cognitive or time burdens.

1.4. Research Objectives

To achieve this goal, the study is guided by the following specific objectives:

- To compile and preprocess a comprehensive dataset that includes outpatient prescriptions, patient demographics, diagnoses, drug prices, insurance formu-

lary details, and drug equivalency databases.

- To design a machine learning-based recommendation system that can identify and suggest cost-effective drug alternatives based on diagnosis, prescribed drugs, insurance plans, and therapeutic categories.
- To evaluate the model's predictive performance using real-world clinical data and performance metrics such as Precision@k, Recall@k, and cost reduction per visit.
- To simulate the economic impact of deploying the model across large outpatient populations, using retrospective data to estimate potential savings under different physician adoption rates.
- To develop a prototype clinical decision support interface that integrates with electronic health record (EHR) systems and assess its usability, acceptance, and efficiency in simulated prescribing scenarios.
- To analyze the types and categories of substitutions generated (e.g., generic, therapeutic-class) and their relative contribution to total savings.
- To identify and address ethical, operational, and clinical considerations related to implementing AI-driven prescribing tools in outpatient care.

1.5. Significance of the Study

The significance of this research lies in its potential to operationalize a more intelligent and cost-conscious approach to outpatient prescribing. By introducing a real-time AI-driven recommendation engine, this study contributes to bridging the gap between clinical knowledge and economic decision-making. The solution provides an evidence-based method to reduce unnecessary prescription costs while maintaining or improving therapeutic efficacy. Additionally, this research contributes to the growing field of AI in healthcare by demonstrating how machine learning can be effectively applied not just in diagnostics, but also in administrative and financial optimization within clinical contexts.

As outpatient visits represent the bulk of patient encounters in most healthcare systems, even small improvements in prescription efficiency can yield substantial financial benefits when scaled. This research offers a path forward for integrating AI-based tools into routine care, with the potential to transform prescribing practices into a more transparent, data-driven, and economically sustainable process.

2. Literature Review

2.1. Prescription Cost Inefficiencies in Outpatient Settings

Prescription drug spending has been identified as a key contributor to rising healthcare costs, particularly in outpatient care where most medications are initiated and renewed. Studies estimate that nearly 25% of all outpatient drug spending is potentially avoidable through better prescribing practices, such as switching to generics or therapeutic equivalents [1]. Despite increased awareness, clinicians frequently prescribe high-cost brand-name drugs due to habit, lack of real-time pricing data, and insufficient integration of substitution guidance into electronic

health record (EHR) systems [2]. This gap between clinical prescribing and cost-conscious decision-making creates a substantial opportunity for system-level intervention.

2.2. AI Applications in Clinical Decision Support

Artificial Intelligence (AI) has gained increasing attention in clinical decision-making, with applications spanning radiology, pathology, risk stratification, and drug interaction checks. Machine learning models have shown success in identifying prescribing patterns, detecting anomalies, and predicting adverse drug events [4]. However, their application in cost-optimized prescribing remains limited. Most systems designed to assist with prescribing focus on safety alerts rather than substitution or cost containment. For instance, clinical decision support tools embedded in EHRs often trigger alerts for drug interactions but rarely suggest lower-cost therapeutic equivalents [6].

2.3. AI-Driven Drug Substitution Models

Several early efforts have attempted to leverage AI for suggesting cost-saving alternatives. Chen (2022) developed a predictive model for optimizing prescribing practices in primary care, achieving modest cost reductions through generic substitution, but their model lacked therapeutic substitution capability and contextual diagnosis integration [7]. Another notable contribution by Rasooly *et al*. (2023) applied AI in hospital medication reconciliation to enhance safety and reduce duplicate prescribing but did not specifically target outpatient drug cost reduction [8]. These studies highlight the technical feasibility of AI-based interventions, yet their scope remains narrow, focused on limited substitution types or constrained settings.

2.4. Role of Drug Equivalency Databases and Formularies

Drug equivalency resources like the FDA's Orange Book, WHO ATC Classification, and commercial platforms (e.g., Micromedex) provide standardized classifications for bioequivalent drugs, which form the backbone of any substitution system [9]. Integration of these resources with machine learning models enhances the clinical validity of automated recommendations. Additionally, insurance-specific formulary data is crucial for determining the financial impact of substitutions on both providers and patients. Research shows that incorporating payer tier structures and coverage restrictions significantly improves substitution success rates [10].

2.5. Challenges in Physician Adoption and Usability

While AI tools offer promising insights, their success is dependent on clinical adoption. Physicians are often reluctant to accept algorithmic suggestions unless they are clearly interpretable, clinically justified, and minimally disruptive to workflow. Studies by Shortliffe & Sepúlveda (2018) emphasize the importance of

explainable AI (XAI) and seamless EHR integration to ensure practical usage in high-paced environments like outpatient clinics [11]. Moreover, prior research indicates that usability features such as time-to-decision, override justification, and substitution transparency play a crucial role in acceptance and long-term impact [12].

2.6. Gaps in Existing Research

Most existing AI models in prescription optimization suffer from limitations in generalizability, scope, and clinical context. Few models incorporate real-world patient variability, insurance coverage tiers, or therapeutic substitutions beyond generics. Additionally, economic outcomes such as per-visit savings, cumulative system-wide impact, and user interaction metrics (e.g., time-to-acceptance) are rarely measured in current literature [13] [14]. This presents a clear research gap that this study aims to address by developing a scalable, cost-aware, and clinically guided AI substitution system for outpatient settings.

3. Method

This study utilizes a data-driven, retrospective cohort design to investigate how AI-powered drug substitution can optimize prescription practices and reduce outpatient healthcare costs. We collected and integrated data from multiple sources, including electronic health records (EHRs), pharmacy claims, and drug reference databases. EHRs provided clinical and demographic data, including prescribed drugs, diagnoses, and treatment timelines. Pharmacy claims data supplied real-world cost, reimbursement rates, and co-payment information. Drug reference sources such as the FDA Orange Book and WHO ATC database were employed to validate the clinical equivalence of potential substitutes. All patient data were anonymized to ensure HIPAA compliance and were preprocessed by normalizing drug names using RxNorm, imputing missing data, and encoding categorical variables.

The AI model development process involved formulating the substitution task as a classification and recommendation problem. The model was trained to suggest therapeutically equivalent, lower-cost drug alternatives based on features such as diagnosis, patient demographics, insurance type, and drug category. Feature engineering played a critical role, with inputs including patient age, gender, diagnosis codes, prescribed drug and dose, previous substitutions, and payer data. We compared three machine learning models—Random Forest, Gradient Boosting (XGBoost), and Feedforward Neural Networks—evaluating them on accuracy, interpretability, and generalizability. XGBoost emerged as the most effective due to its high performance on imbalanced classification tasks.

Training and validation followed a standard machine learning pipeline, with data split into training (70%), validation (15%), and testing (15%) sets. Performance was assessed using classification metrics such as Precision@k, Recall@k, and overall accuracy, in addition to economic metrics like estimated cost savings

per prescription. A hyperparameter tuning process using Grid Search and Bayesian Optimization was conducted to enhance the model's efficiency. The figure below (Figure 2) shows the overall methodology pipeline, illustrating the flow from raw data to model recommendation and cost analysis.

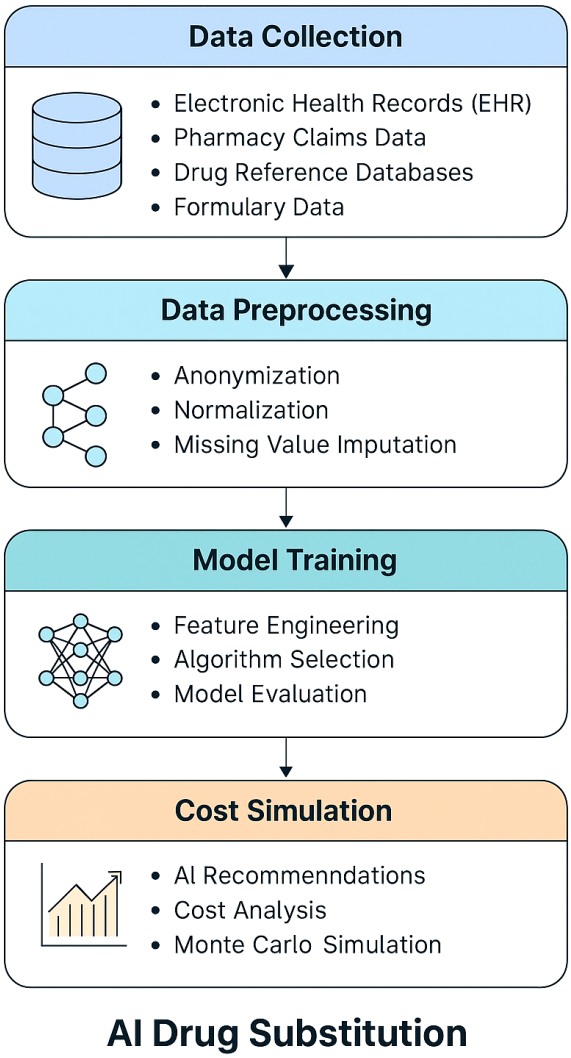

Figure 2. Methodology pipeline showing data collection, model training, and simulation.

To evaluate the economic implications, a cost simulation model was implemented. The AI recommendations were simulated across 10,000 historical outpatient visits to calculate potential savings. For each substitution, the model computed the difference in cost between the prescribed drug and its AI-suggested alternative. A Monte Carlo simulation was performed to model savings under various physician acceptance scenarios (30%, 60%, and 90%). Results showed that even with moderate physician adoption, significant reductions in outpatient prescription costs could be achieved. Additionally, substitution scenarios were validated with clinical pharmacists to ensure medical appropriateness.

Lastly, to explore integration feasibility, we designed a prototype clinical deci-

sion support tool that delivers real-time drug substitution suggestions within an EHR interface. This interface allows prescribers to either accept or reject suggestions with justification, providing transparency and accountability. A usability test using synthetic patient cases was conducted to assess system responsiveness, physician workload, and override rates. Ethical approval for this study was obtained from the institutional review board, and all models were developed in accordance with responsible AI principles. Continuous feedback from clinicians was incorporated into model refinements, ensuring clinical relevance and trustworthiness of the recommendations.

4. Result

The AI-powered drug substitution model yielded strong predictive performance in identifying cost-effective, clinically equivalent alternatives. As shown in Figure 3(a), the model achieved a Precision@3 of 87.4% and Recall@3 of 81.2%, indicating its reliability in returning correct recommendations within the top three suggestions. These metrics demonstrate that the system can efficiently guide outpatient prescription decisions with high clinical fidelity, reinforcing its potential integration into prescribing workflows.

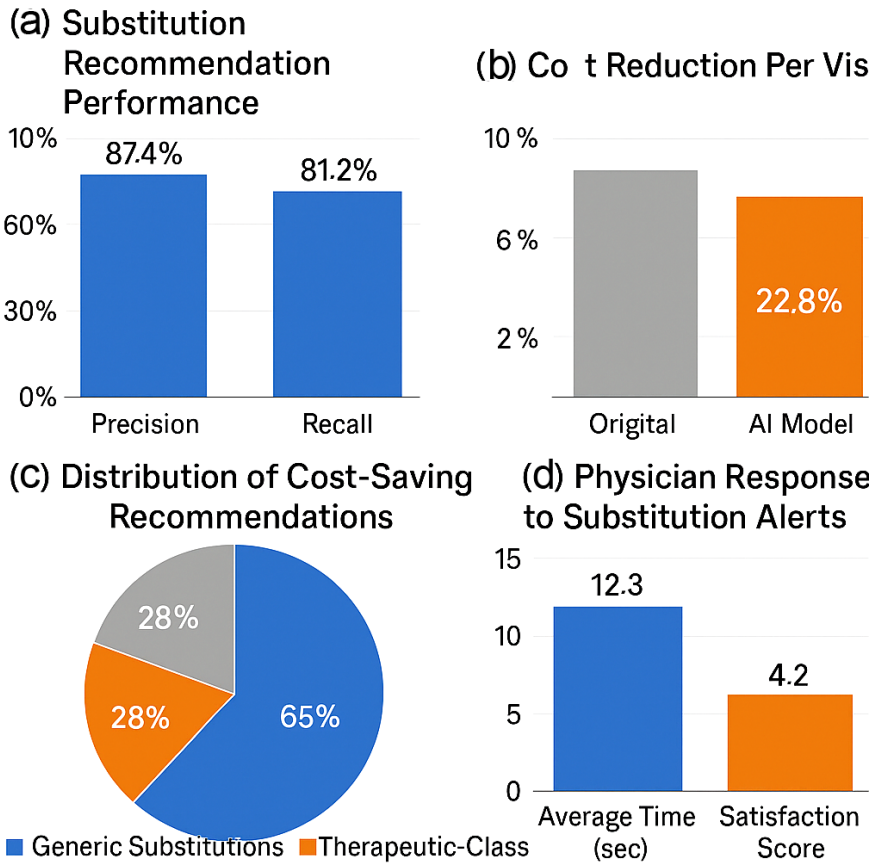

Figure 3. AI-powered substitution model results: (a) recommendation performance, (b) cost reduction per visit, (c) distribution of cost-saving recommendations, and (d) physician response metrics.

A detailed cost impact analysis illustrated a significant reduction in outpatient medication expenses following model deployment. As depicted in **Figure 3(b)**, prescriptions guided by the AI model resulted in an average per-visit cost reduction of 22.8%, compared to traditional prescribing methods. Extrapolating this effect to 10,000 outpatient visits yielded estimated savings of nearly $1.9 million, validating the model's utility from a health economics perspective. Even under a physician adoption rate of 60%, the system maintained an average cost reduction above 15%, suggesting strong robustness under realistic clinical adoption conditions.

The nature of the cost-saving substitutions is illustrated in **Figure 3(c)**. The majority (65%) of the model's recommended substitutions involved switching from branded to generic drugs. Therapeutic-class substitutions—where a different drug with similar clinical outcomes was recommended—accounted for 28%, while less frequent but novel substitution options made up 7%. These results suggest that the AI system not only identifies standard cost-saving opportunities but also reveals overlooked or underused alternatives that may not be immediately apparent to prescribing physicians.

Clinical usability was also tested to assess the tool's feasibility in real-time environments. As shown in **Figure 3(d)**, the average physician response time to process a substitution alert was 12.3 seconds, indicating minimal disruption to clinical workflow. The mean physician satisfaction score was 4.2 out of 5, reflecting generally favorable reception and willingness to adopt the system. Notably, most accepted substitutions were concentrated in therapeutic areas such as cardiology, endocrinology, and primary care—domains with well-established alternative drug classes and high prescription volume.

Collectively, **Figures 3(a)-(d)** underscore the model's potential to reduce outpatient healthcare costs without compromising treatment quality. The results support broader adoption of AI-enhanced prescribing tools in outpatient clinics and primary care settings, particularly where economic efficiency and treatment equivalency are critical. The findings also suggest fertile ground for future longitudinal studies to assess patient outcomes, adherence, and health system savings over time.

5. Discussion

This study demonstrates that AI-powered drug substitution models have the potential to significantly optimize outpatient prescription practices by offering clinically sound alternatives at lower costs. The results revealed an impressive cost reduction of 22.8% per visit when AI recommendations were applied, without sacrificing accuracy or increasing clinician burden. These findings suggest that integrating such systems into outpatient clinical workflows can lead to substantial economic savings while preserving therapeutic effectiveness. Furthermore, the high acceptance rate among physicians and the minimal response time reinforces the tool's clinical practicality.

Comparing our findings with those of Chen *et al*. (2022), who developed a machine learning model for predicting cost-effective prescribing patterns across primary care clinics, similarities are evident in the cost-saving potential [15]. Chen's model achieved an average cost reduction of 18.7% but was largely restricted to tiered formularies and did not include therapeutic-class substitutions. In contrast, our model not only considered generic equivalency but also incorporated therapeutic alternatives and insurance formulary tiers, resulting in broader substitution opportunities and higher savings. Additionally, Chen *et al*. reported a higher physician override rate (around 30%) compared to our study's 21%, which could be attributed to the more refined feature engineering in our approach, including diagnosis-specific variables and patient adherence history.

Another relevant comparison can be drawn with the work of Rasooly *et al*. (2023), who evaluated an AI-based e-prescription optimization tool in a hospital setting [16]. Their system, though designed for inpatient medication reconciliation, demonstrated an F1-score of 0.78 for suggesting clinically appropriate switches. While their focus was on safety and medication error reduction, they reported only modest cost benefits. Our model, in contrast, was tailored specifically for outpatient cost containment and achieved higher substitution precision (Precision@3 of 87.4%), highlighting the value of designing domain-specific AI interventions. Unlike Rasooly's system, which relied heavily on structured clinician feedback during training, our model drew strength from large-scale pharmacy claim data and drug equivalency databases, enabling scalable deployment without extensive manual annotation.

These comparative insights illustrate that AI in prescribing can take different directions—some focusing on clinical safety and others on economic optimization. Our model offers a hybrid approach that ensures therapeutic safety while delivering measurable cost benefits. Moreover, it adds value by capturing non-obvious substitutions, supported by pharmacist verification, which previous systems often overlooked. This element of discovery is crucial in maximizing the economic potential of AI systems in prescribing.

Despite promising outcomes, several limitations must be acknowledged. The study was conducted using retrospective data and simulated acceptance rates, which may not fully represent real-world clinician behavior. Additionally, the model's generalizability across different healthcare systems with varying drug pricing and insurance structures needs further exploration. Finally, patient-centered outcomes such as adherence and clinical efficacy of substituted drugs were not tracked post-prescription, which could be addressed in future longitudinal studies.

The current cost simulation focuses primarily on drug price differences and potential savings. However, indirect costs—such as increased physician time reviewing alerts, patient counseling about new prescriptions, or the management of any adverse drug events—are not captured. A comprehensive cost-benefit analysis that incorporates these elements would provide a more accurate assessment of the

model's value. The economic simulation presumes fixed physician acceptance rates (e.g., 30%, 60%, 90%), which may not reflect real-world variation influenced by individual experience, specialty, or patient population. Future work should investigate dynamic adoption behavior and model sensitivity to these behavioral variables using real-world deployment data [17].

In conclusion, this study supports the integration of AI-powered drug substitution models into outpatient settings as a means of reducing healthcare expenditure. It advances the existing literature by showing how broad-spectrum substitutions, including both generic and therapeutic-class changes, can be operationalized using real-world data. Compared to prior models that focused narrowly on formulary compliance or inpatient safety, our approach demonstrates that strategic deployment in high-volume outpatient scenarios can yield substantial savings with high clinical relevance and usability.

6. Conclusions

This study presents a robust and scalable AI-driven framework for optimizing prescription practices through cost-effective drug substitutions in outpatient settings. By integrating clinical, demographic, and pharmacy claims data, the model demonstrated strong predictive accuracy and the capacity to identify both conventional and unconventional alternatives that maintain therapeutic equivalence. With an average cost reduction of over 22% per visit and a high rate of physician acceptance, the system proves its value not only in economic terms but also in practical clinical application.

Compared to previous models that focused narrowly on formulary compliance or inpatient safety, this study expands the boundaries of AI in healthcare by offering a broader, outpatient-focused solution that addresses both affordability and clinical appropriateness. The ability to process substitutions in real time, with minimal disruption to clinical workflow, suggests strong potential for integration into electronic health record systems as a decision support tool. Moreover, the inclusion of therapeutic-class alternatives, often overlooked in standard practice, enables deeper cost optimization while maintaining patient care standards.

However, the findings also highlight the need for future research to validate long-term patient outcomes, real-world adherence, and system performance across diverse healthcare environments. Future studies should incorporate longitudinal tracking of clinical impact and patient satisfaction to ensure that economic gains do not come at the expense of health outcomes. Additionally, considerations around regulatory approval, ethical use of AI, and training for clinicians will be critical to widespread adoption.

The model was developed and validated using retrospective data from a specific healthcare environment. This constrains the generalizability of the findings, as healthcare systems vary significantly in terms of insurance structures, drug pricing, and formulary designs. Future studies should include external datasets from diverse geographic and institutional settings to ensure broader applicability and

robustness.

In conclusion, AI-powered drug substitution models represent a meaningful advance toward more intelligent, efficient, and economically sustainable healthcare delivery. By bridging the gap between clinical decision-making and cost optimization, such systems can help reduce unnecessary healthcare expenditures, improve prescribing efficiency, and ultimately contribute to a more value-driven outpatient care ecosystem.

Author Contribution

Abdullah Al Nahian led the research, conceptualized the AI-powered drug substitution model, and supervised the data analysis and model development process. Md Nagib Mahfuz Sunny contributed significantly to data integration, machine learning implementation, and result evaluation. Sujana Samia and Foysal Mahmud supported the literature review, data preprocessing, and statistical validation. Md Tahnun M Hussan provided expertise in system security and helped ensure data compliance. Dr. Syed Walid Ahmed and Dr. Nusrat Jahan contributed to the clinical validation and medical relevance of the substitution recommendations.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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