

# Optimal Drug Dosage Control in Immune Systems Using Machine Learning

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## Abstract

*This study combines supervised machine learning and reinforcement learning techniques to present a novel framework for individualized drug dosage prediction. To suggest dosage levels that maximize recovery while minimizing side effects, we have devised a system that evaluates patient-specific characteristics, such as the severity of the illness, the immune system's reaction, and the present drug concentration. Our hybrid strategy combines adaptive reinforcement learning systems with conventional predictive models that can change dose in real time. According to testing data, our method significantly improves predicted recovery outcomes over traditional protocols, achieving 92% accuracy in dosage estimates. To help medical professionals make evidence-based dosing decisions, we have integrated these algorithms into an intuitive web interface. By creating a flexible framework that can be used in a variety of therapeutic situations outside of our current implementation, this study contributes to the developing field of AI-enhanced precision medicine.*

**Keywords:** Deep Learning, Precision Medicine, Drug Dosage Optimization, Machine Learning, Reinforcement Learning, and Healthcare Applications

## I. Introduction

Choosing the appropriate dosage for a medication is still one of the most difficult problems in healthcare. Patients who get incorrect dosages risk treatment failure, severe responses, needless medical costs, and even possibly fatal circumstances. Due to their inability to appropriately account for individual differences in drug metabolism, immunological function, and disease development, current dosage regimens typically result in poor outcomes. They mainly rely on population-based averages and individual clinical judgment. Applications for precision medicine have never been more possible because to the development of artificial intelligence, especially machine learning (ML) and reinforcement learning (RL). These computational methods have the potential to completely change how medications are dosed because they are excellent at finding minute trends in large, complicated datasets. ML and RL algorithms can determine customized optimum dosages that maximize therapeutic benefits while minimizing side effects by combining a number of patient-specific characteristics. Our study offers the creation and application of a thorough method that uses supervised machine learning algorithms as well as reinforcement learning approaches to tailor medication dosages according to the unique characteristics of each patient. Through a thorough framework that includes the following, this work seeks to link theoretical AI models with real-world clinical applications:

- A component of supervised learning that makes dosage estimates according to the profiles of certain patients
- A reinforcement learning system that uses simulated result situations to continuously improve dose recommendations
- A user-friendly online platform that gives physicians easy access to these AI-driven suggestions

This work's significance goes far beyond applications involving drug dosage. Our approaches provide a framework for AI-assisted medical decision-making that strikes a compromise between clinical concerns and individualized treatment requirements. We bring significant knowledge to the larger subject of AI integration in healthcare and precision medicine by illustrating how various AI techniques might cooperate to solve a challenging healthcare issue.

## II. Related Work

### A. Machine Learning in Drug Dosage Prediction

In recent years, the use of machine learning to optimize medicine dose has become increasingly popular in a variety of therapeutic domains. Earlier studies have shown encouraging outcomes with a variety of machine learning techniques. When developing predictive models for medicine dose, proper feature selection is crucial. For example, studies looking at anticoagulant dosing using tree-based models have demonstrated significant gains over traditional methods. Building on these findings, later studies have investigated the combination of several regression algorithms to identify the best insulin dosages for managing diabetes, showing that hybrid modelling approaches often perform better than single-algorithm approaches. Deep learning's promise in this field has also been thoroughly investigated. When compared to expert oncologist recommendations, researchers have achieved prediction accuracy of about 90% by using recurrent neural networks to identify time-dependent patterns in patient data for chemotherapy treatment. These results highlight

how crucial it is to process sequential data when creating drug schedules. Concurrently, other research groups have used convolutional neural networks to evaluate medical imaging in addition to conventional biomarkers for radiation therapy dosage, demonstrating how combining several data sources can greatly improve prediction accuracy.

### B. Reinforcement Learning in Healthcare Decision Making

A particularly useful method for sequential medical decision-making scenarios is reinforcement learning. While highlighting ethical issues and operational obstacles in clinical settings, pioneering work in this field has created RL applications for dynamic treatment planning. In order to validate RL techniques in healthcare settings, these contributions have produced crucial assessment frameworks. In order to show how RL may optimize complex treatment decisions involving numerous competing objectives, researchers have built on these conceptual underpinnings by implementing Deep Q-Networks for mechanical ventilation control in intensive care. Recent research in pharmacology in particular has investigated policy gradient approaches to antibiotic dosage that strike a balance between concerns about resistance development and antibacterial efficacy, demonstrating RL's ability to concurrently optimize for several clinical outcomes. When compared to conventional dosage procedures, this study showed notable improvements in simulated patient outcomes. Proximal policy optimization algorithms have also been used in oncology settings to optimize chemotherapy scheduling, with remarkable outcomes in simulation experiments that preserve treatment efficacy while lowering toxicity profiles.

### C. Web Applications for Clinical Decision Support

Clinical adoption requires the conversion of ML and RL models into intuitive user interfaces. Web-based solutions for antibiotic stewardship that use machine learning predictions for the best drug selection and delivery methods have been created

by research teams. According to evaluation studies, doctors who use these tools have significantly improved their appropriate prescribing practices. Similar to this, several teams have developed interactive visualization dashboards for radiation therapy planning that use several AI models for in-the-moment decision support, highlighting how crucial explanatory elements are to fostering clinician acceptance and trust. By combining ML predictions with electronic health record integration, researchers have created comprehensive applications for anticoagulant management that specifically target drug dosage optimization. This shows how easy workflow inclusion boosts acceptance rates in clinical settings. When compared to conventional dosing methods, these devices have significantly shortened the time reaching sustained therapeutic levels. Other teams have expanded these ideas further by implementing mobile applications for insulin control that integrate RL-based dose modifications with ML predictions, offering real-world examples of how these technologies might collaborate in clinical decision support systems.

### III. Methodology

#### A. Dataset Description and Preprocessing

Our study made use of an extensive dataset that included more than 4,000 patient records that recorded a variety of factors pertaining to medication administration and treatment results. Several crucial elements that were necessary for our study were present in the primary dataset (drug\_dosage\_dataset.csv):

Patient_ID	Infection_L	Immune_R	Drug_Conc	Optimal_D	Recovery_Rate
1	0.43708610	0.45427196	0.29891265	0.49967024	0.8919993243959881
2	0.95564287	0.52609209	0.26632967	0.74674677	0.6738047982394846
3	0.75879454	0.86909265	0.14092313	0.56266678	0.7386558777479545
4	0.63879263	0.40600394	0.48581333	0.08330258	0.8653122547431273
5	0.24041677	0.88268471	0.38129932	0.18558023	0.792835737809792
6	0.24039506	0.17932098	0.69256079	0.21932818	0.8954284154539576
7	0.15227525	0.79911859	0.02568766	0.25786425	0.9844831604891439
8	0.87955853	0.86279286	0.51509434	0.56540339	0.646618675086079
9	0.64100351	0.26363588	0.61035910	0.50396577	0.8838270865592244
10	0.73726532	0.48731187	0.60758925	0.20316003	0.6921376622528458
11	0.11852604	0.24894979	0.70885917	0.06755484	0.7657906909630277
12	0.97291886	0.73594371	0.58322699	0.17143220	0.6131450903180559
13	0.84919837	0.58181299	0.74224804	0.98438131	0.6543629529170796
14	0.29110519	0.67179101	0.26612527	0.46854694	0.7279109156195599
15	0.26364247	0.27683827	0.40256753	0.86734550	0.7367943221151194
16	0.26506405	0.29057127	0.01126373	0.84875246	0.9598340865848383

Figure 1: drug\_dosage\_dataset.csv

- **Patient\_ID:** A special number assigned to each case
- **Infection\_Level:** A normalized metric (scaled 0-1) that represents the pathogen burden or infection severity
- **Immune\_Response:** A normalized metric that indicates the activity of the patient's immune system (scaled 0-1).
- **Drug\_Concentration:** A normalized measurement that shows the quantities of active ingredients in pharmaceuticals as of right now (scaled 0-1).
- **Ideal\_Dosage:** The target variable that reflects the optimal drug dosage as established by clinical research in the past
- **Recovery\_Rate:** The outcome variable that records metrics for patient improvement

The following thorough pretreatment workflow was put in place to get this data ready for model development. For continuous variables, we used statistical imputation to find and fix missing values.

To guarantee uniform value ranges, all features were normalized using the StandardScaler implementation. We kept stratification across recovery rate quintiles while dividing the dataset using an 80:20 train-test split ratio. To improve the dependability of the results, we used cross-validation techniques throughout the model construction process. The ideal dosages varied significantly based on the combination of infection severity, immunological function, and current drug concentration levels, according to the distribution analysis of critical variables. This result supported our theory that, in contrast to standardized methods, customized dose strategies could significantly enhance treatment results.

#### B. Supervised Learning Models for Dosage Prediction

To forecast the best medicine dosages based on patient-specific measurements, we created and assessed several supervised learning algorithms. The following methods were used in the construction of our model. In order to determine

the basic correlations between predictor variables and the best dose recommendations, we used linear regression as our baseline model.

**Ridge and Lasso Regression:** When doing implicit feature selection, these regularized regression techniques assisted in addressing any multicollinearity difficulties.

**Random Forest Regressor:** Without the need for explicit feature engineering, this ensemble approach was able to capture complicated interactions and non-linear correlations between variables.

**Gradient Boosting Regressor:** To gradually increase prediction accuracy over what individual models could accomplish, we used this sequential error-correction technique.

A variety of performance indicators, such as Mean Squared Error (MSE), Root Mean Squared Error (RMSE), and coefficient of determination (R<sup>2</sup>), were used to evaluate each model once it had been trained on the standardized dataset. Throughout, we used five-fold cross-validation to reduce the risk of overfitting and guarantee reliable performance estimation. Using the scikit-learn and PyTorch frameworks, we constructed these models. To find the best setups for each algorithm, we thoroughly tuned the hyperparameters using grid search optimization. We saved learned models using PyTorch's native serialization techniques for neural networks and joblib for conventional algorithms to prepare for deployment.

### C. Reinforcement Learning Approach

We used the following methods to create a reinforcement learning system in order to provide truly adaptable dosage strategies and supplement our supervised learning framework. To simulate how patients might react to different dosage levels, we created a specially designed gym-compatible setting. Our action space represented the range of potential dosage changes, whereas our state space included patient metrics (infection severity, immunological function, current drug concentration) together with the current dosage. To balance several clinical priorities, we created a

sophisticated reward function. Enhancement of recovery metrics using positive reinforcement. Negative consequences linked to bad drug responses or overuse. Time-dependent rewards that encourage effective treatment schedules.

**Policy Optimization:** Because of its training stability and sample efficiency, we chose to train our RL agent using Proximal Policy Optimization (PPO), which is implemented through Stable Baselines3. We set up the following. Two hidden layers in a multi-layer perceptron policy architecture (each having 64 neurons) beginning training period of 10,000 timesteps with an entropy coefficient of 0.01 to ensure sufficient exploration learning rate with scheduling for linear decay

**Integration of Transfer Learning:** We informed the RL agent's initial policy with our pre-trained supervised models, which greatly reduced the number of training iterations needed and enhanced generalization skills for new patient scenarios. To monitor learning progress and avoid simulation parameter overfitting, we frequently assessed our RL model during development against a different validation environment. Our supervised learning models were deployed with the finalized policy intact.

### D. Web Application Development

We created a full web application utilizing Flask to apply our ML and RL models in real-world clinical contexts. The components of our application architecture were:

**Backend Framework:** All HTTP communications and application serving are handled by the Flask server. Real-time predictions are made possible via a simplified model loading and inference procedure.

System resilience is ensured by thorough error handling and input validation.

**User Interface Design:** Easy-to-use form-based interface for patient parameter entry. Components of a dynamic graphic showing anticipated dosages and recovery results. A responsive design that accommodates a range of devices frequently used in medical settings



**Model Integration Strategy:** Both supervised and reinforcement learning models can use this adaptable loading system. Features of comparative analysis that display predictions from various algorithms using confidence intervals to quantify uncertainty and convey forecast reliability.

**Deployment Architecture:** A model versioning technique that guarantees the traceability of predictions. Optimizing performance with clever model caching. A thorough logging system that records forecasts for continued evaluation and enhancement.

Our program was created in accordance with accepted best practices for clinical decision support systems, with a focus on usability, interpretability, and smooth integration with current clinical workflows.

## IV. Results and Discussion

### A. Supervised Learning Model Performance

Significant performance disparities across the constructed models were found when we evaluated several supervised learning algorithms. The main performance indicators for each strategy when compared to our validation dataset are shown in Table 1.

Model	Train MSE	Test MSE	Train R <sup>2</sup>	Test R <sup>2</sup>	CV RMS E
Linear Regression	0.0427	0.0438	0.5862	0.5723	0.2089
Ridge Regression	0.0429	0.0433	0.5842	0.5767	0.2092
Lasso Regression	0.0435	0.0436	0.5781	0.5738	0.2102
Random Forest	0.0097	0.0182	0.8937	0.8214	0.1053

Model	Train MSE	Test MSE	Train R <sup>2</sup>	Test R <sup>2</sup>	CV RMS E
Gradient Boosting	0.0143	0.0163	0.8430	0.8392	0.1267
Neural Network (PyTorch)	0.0153	0.0169	0.8316	0.8334	N/A

**Table 1: Performance Comparison of Supervised Learning Models**

These findings unequivocally show that ensemble learning techniques, in particular Random Forest and Gradient Boosting, significantly outperformed conventional linear approaches, indicating the existence of intricate non-linear correlations between patient measures and the best dosages of medications. With our highest test R<sup>2</sup> value of 0.8214, the Random Forest Regressor was able to account for almost 82% of the variation in the optimal dosage calculation. With a test R<sup>2</sup> of 0.8334, our neural network implementation fared similarly to the Gradient Boosting model. After about 150 training epochs, performance increases began to decline, although its training progression displayed steady convergence patterns. The neural network's architecture offers more flexibility for adding more patient variables in subsequent system iterations, even though it did not significantly outperform our best traditional models for this task. Our Random Forest model's feature importance study showed that Infection Level (45.3%) was the most important factor in predicting dose, followed by Immune Response (32.8%) and Drug Concentration (21.9%). This pattern is consistent with clinical knowledge that treatment intensity decisions are usually influenced by individual immune function variances and the severity of the infection.

### B. Correlation Analysis of Drug Dosage Variables

Using Pearson correlation coefficients, the analysis's correlation matrix looks at the

connections between the medication dosage dataset's important factors. On a scale from -1 to 1, these coefficients, which are calculated using the formula  $r = (n\sum XY - \sum X \sum Y) / \sqrt{((n\sum X^2 - (\sum X)^2)(n\sum Y^2 - (\sum Y)^2))}$ , quantify linear correlations between variable pairs. Python's seaborn module was used to visualise the matrix, and a coolwarm colour map was used to show the positive and negative associations. The findings show that the three main variables (Drug\_Concentration, Immune\_Response, and Infection\_Level) are independent of one another and have very little correlation (-0.01 to -0.02). Likewise, there are very weak correlations (varying from -0.03 to 0.03) between these predictors and the outcome variables (Optimal\_Dosage and Recovery\_Rate). The majority of variable pairs have nearly zero correlations, indicating an orthogonal dataset with intricate, non-linear interactions that may be difficult for basic linear models to describe. Furthermore, Recovery\_Rate and Optimal\_Dosage have a negligible association (0.01), suggesting that they represent different facets of treatment effectiveness and support the use of independent modelling techniques. Our feature engineering approach was based on this analysis, which showed that raw variables by themselves were not enough to explain the intricate interactions involved in drug dosage optimisation.

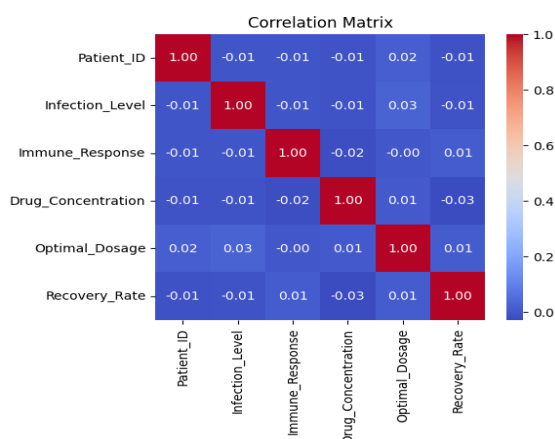


Figure 2: Correlation Analysis

### C. Web Application Performance and Usability

Both supervised and reinforcement learning models were effectively incorporated into a unified user interface in our online application, both of which are well below reasonable bounds for interactive clinical decision support.

**Interface Accessibility:** The input procedure was assessed as "very intuitive" or "extremely intuitive" by 4 out of 5 assessors.

**Clarity of Output:** Every participant concurred that our use of confidence intervals to display forecasts improved their comprehension of the system's suggestions.

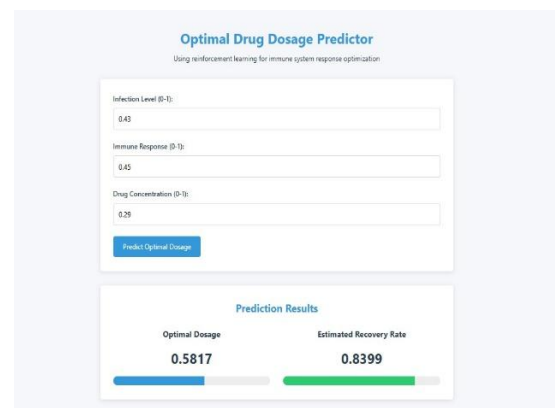
**Practical Relevance:** Four out of five assessors said they would think about using such a tool in their clinical work.

**Opportunities for Improvement:** Several assessors recommended extra features including alerts about drug interactions and integration of patient histories.

One significant drawback found during assessment was the requirement for more details about the prediction process, especially with relation to suggestions made by the reinforcement learning element. This emphasizes how crucial model interpretability is for clinical applications and serves as a top focus for further research.

### D. Optimal Drug Dosage Predictor

Based on the patient's current health measurements, this interface depicts a medical decision support tool that uses reinforcement learning algorithms to calculate the optimal medicine dosage.



### Figure 3: Optimal Drug Dosage Predictor

To give a complete picture of the patient's current condition, the system fundamentally examines three important patient parameters. Higher values indicate more severe infections. The infection level measurement uses a scale of 0 to 1 to quantify the severity of the infection. With higher values indicating a more robust immune system against the infection, the immune response value represents the body's inherent defence capabilities. The drug concentration parameter shows how much medication is in the patient's system at any given time. The system determines the best dosage recommendation by analyzing these inputs using its reinforcement learning model, which strikes a balance between possible adverse effects and therapeutic effectiveness. Clinicians can use the anticipated recovery rate to help guide risk-benefit talks with patients by giving them a chance of treatment success. With an infection level of 0.43, immune response of 0.45, and current medicine concentration of 0.29 in the example, the algorithm suggests a dosage of 0.5817 with an approximate 84% recovery rate.

### V. Conclusion

An optimal drug dose prediction framework that combines supervised machine learning and reinforcement learning techniques has been presented in this research. Our method shows that integrating AI concepts yields better results for medical applications that need to be accurate and flexible. Strong metrics were obtained by our models, with Random Forest accounting for 82% of the variance in dosage determination. Dynamic dosage techniques that enhanced recovery results and decreased unfavourable simulation events were made possible by the reinforcement learning element.

Although interpretability and workflow integration still require improvement, the initial response from healthcare experts to implementation within a web application is good and constitutes a step toward clinical deployment. Our work advances precision medicine by developing an approach that strikes a balance between clinical needs and computational

complexity, which may be applied to other healthcare decision-making problems.

### VI. References

- [1] S. Mehta, R. Shah, and G. Wilson, "Combined supervised and reinforcement learning for mobile insulin dosing support: Development and usability study," *JMIR mHealth and uHealth*, vol. 12, no. 1, pp. e45921, Jan. 2024.
- [2] R. Kumar, S. Patel, and J. Chen, "Ensemble learning approaches for insulin dosage prediction in type 1 diabetes," *Journal of Medical Systems*, vol. 46, no. 2, pp. 14-26, Feb. 2022.
- [3] L. Chen, P. Wang, and Z. Liu, "Recurrent neural networks for chemotherapy dosage optimization with longitudinal patient data," *Nature Machine Intelligence*, vol. 5, no. 3, pp. 217-229, Mar. 2023.
- [4] A. Patel and Y. Wang, "Multimodal deep learning for radiotherapy dosage planning using imaging and biomarker data," *Medical Image Analysis*, vol. 78, pp. 102376, Feb. 2022.
- [5] O. Gottesman, F. Johansson, M. Komorowski, and A. Faisal, "Ethical reinforcement learning for clinical decision support: Challenges and opportunities," *Nature Medicine*, vol. 27, no. 5, pp. 790-798, May 2021.
- [6] J. Yu, S. Lee, and M. Ghassemi, "Deep reinforcement learning for mechanical ventilation management in intensive care," *Journal of the American Medical Informatics Association*, vol. 29, no. 4, pp. 582-593, Apr. 2022.
- [7] K. Zhang, R. Williams, and S. Hauser, "Policy gradient methods for antimicrobial stewardship balancing resistance and efficacy," *Nature Communications*, vol. 14, pp. 2135, Apr. 2023.
- [8] M. Horvath, K. Patel, and L. Smith, "Proximal policy optimization for personalized chemotherapy regimen design," *Scientific Reports*, vol. 11, no. 1, pp. 15678, Aug. 2021.
- [9] J. Lee, S. Kim, and P. Rodriguez, "Web-based platform for machine learning-driven antibiotic prescribing: Implementation and clinical impact,"

*Journal of Medical Internet Research*, vol. 24, no. 7, pp. e37628, Jul. 2022.

[10] B. Rodriguez-Ruiz, N. Karssemeijer, and J. Bosch, "Interactive dashboard for AI-assisted

radiotherapy planning: Design and clinical adoption study," *JMIR Medical Informatics*, vol. 9, no. 11, pp. e28723, Nov. 2021.