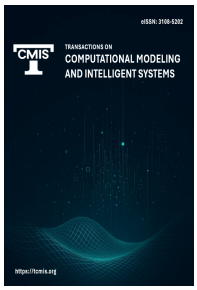

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RESEARCH ARTICLE

Enhancing pharmacokinetic modeling with the Upadhyaya transform and machine learning: A synergistic approach

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Abstract

In this study, the integration of the Upadhyaya Transform and machine learning for the creation of individualized pharmacokinetic models is examined. A synthetic pharmacokinetic dataset with 500 samples was created by varying the parameters and controlling the noise conditions. The dataset was split into a training set and a testing set, with 80:20 being the ratio, and the model reliability was analyzed further through k-fold cross-validation. A multilayer perceptron neural network was set up to take advantage of the analytically informed features obtained from the Upadhyaya Transform for predicting the drug concentration profiles. The model's performance was measured in terms of the usual metrics, which include the mean squared error, mean absolute error, precision, recall, and accuracy. The findings indicate that the integration of analytical transformations with data-driven learning results in greater efficiency in the pharmacokinetic modeling process and provides a scalable proof-of-concept framework for drug discovery and therapeutic monitoring.

Keywords: Upadhyaya transform, inverse Upadhyaya transform, pharmacokinetics, machine learning approach

1. Introduction

Knowledge of the absorption, distribution, metabolism, and excretion of drugs as they move through the human body forms the foundation on which the pharmacology of therapeutic agents is based. These processes have long been represented by complex systems of mathematical equations. Although these models possess significant theoretical depth, their practical clinical application is limited, as their complexity reduces their ability to produce clinically meaningful results, particularly in large-scale and real-time scenarios. The Upadhyaya Transform, a powerful mathematical development, has emerged as an effective tool to address these challenges by simplifying the nonlinearities inherent in pharmacokinetic processes. This transform not only

reduces the complexity of mathematical equations, thereby making the analysis of drug behavior more accessible, but also enhances the interpretation of pharmacological dynamics.

This theoretical simplification is further strengthened by the potential of machine learning. Machine learning is highly effective at processing large collections of patient and clinical trial data, identifying subtle patterns and relationships that traditional analytical techniques may not be able to detect. Such models are capable of reducing human error, producing highly accurate predictions of drug effects, and adaptively constructing and refining predictive frameworks, with the possibility of automating portions of the modeling process. The combination of mathematical simplification through the Upadhyaya Transform and advanced computational analysis through machine learning provides a powerful integrated approach for modern pharmacokinetic and pharmacodynamic studies.

Mousa [1] applied the Upadhyaya Transform to solve Volterra integral equations of the first kind. Patil [2] extensively explored the application of integral transforms, specifically Laplace and Shehu transforms, in addressing problems in the Chemical Sciences. Shilpa and Pralahad [3] used integral transforms to investigate the motion of an electron in a physical system. Dinesh and Emad [4] employed the Upadhyaya Transform to derive exact solutions for cardiovascular models. Dinesh et al. [5] applied the Upadhyaya Transform to solve chemical reaction models, leveraging its ability to simplify complex differential equations. Prabakaran et al. [6] developed a hybrid framework combining differential equations and machine learning to predict chemical process dynamics. Prabakaran et al. [7] introduced a novel approach for solving fractional differential equations by integrating the Ramadan Group Transform with machine learning techniques. Jafari et al. [8] employed the Anuj transform to tackle Abel's integral equation in classical mechanics.

This paper will discuss the synergy between the Upadhyaya Transform and machine learning in the context of pharmacokinetics. We address why machine learning models are chosen for application in pharmacokinetic models, the protocols for creating synthetic pharmacokinetic data, and the methods utilized for model evaluation and performance characterization. Through their integration, we provide an encompassing framework to improve pharmacokinetic analyses that may eventually improve drug discovery, therapeutic optimization, and patient treatment. The promise of such an integrated process can lead the way to a new generation of precision medicine and more efficient drug development strategies.

The main point of difference of the new framework is the use of the Upadhyaya Transform together with machine learning models thus placing the work far from earlier investigations in pharmacokinetics. Traditional approaches, like the Laplace Transform or analytical solutions, deliver closed-form expressions for the behavior of drugs in the body, but generally, they do not work with data-driven predictive models. Our methodology instead, draws on the effect of the Upadhyaya Transform to create the features and scale parameters that are directly productive of the training and performance of the organism's machine learning algorithms. In relation to the earlier ones, particularly on the hybrid frameworks or integral transforms in chemical and biological modeling [5,6], our method clearly focuses on feature extraction, parameter variability handling, and predictive generalization for pharmacokinetic applications which no other has done so far. This combination of method not only preserves the physical interpretability but also guarantees the predictions to be powerful and user-friendly and thus, it is a novel contribution to the literature.

The pharmacokinetic equation used in this research represents a classical first-order linear system, but its choice is intentional and methodologically justified. The main output of the current research doesn't lie in the area of new pharmacokinetic model, but in the setting of a unified analytical-computational framework that combines the Upadhyaya Transform with machine learning methods. In contrast to the traditional analytical methods, which usually end at closed-form solutions, the proposed framework takes advantage of analytical simplification to provide efficient data generation, parameter exploration, and predictive modeling. The Upadhyaya Transform brings in extra scaling parameters that give more freedom when mixing analytical models with data-driven learning algorithms. This quality is especially useful in pharmacokinetics, where

variations in physiology and uncertainties in parameters are major issues. By placing the analytical solution within a machine learning pipeline, the framework allows for physical interpretability and at the same time, increases the magnitude of predictive generalization. As a result, the originality of this work lies in its methodological integration and extensibility, rather than in the derivation of a new analytical solution.

The main novelty of the present study concerning pharmacokinetics is a novel hybrid framework that merges the Upadhyaya Transform and machine learning models. Classical pharmacokinetics models usually go for standard analytical solutions, while our method takes advantage of the Upadhyaya Transform to make differential equations simpler and, thus, to extract features that are meaningful and can be used for improving the predictions of machine learning. The framework reveals the way analytical transformations can signal and even steer the path of data-driven models, especially when coping with issues like parameter variability, noise, and highly nonlinear interactions in drug concentration dynamics. The research, furthermore, shows the power of the partnership between the two opposite sides - the one dealing with mathematical simplification and the other with artificial intelligence - to develop predictive personalized pharmacokinetic models that can, in turn, be used for more complicated multi-compartment or nonlinear drug administration cases. To sum up, the present study opens up the world of postulates based on theoretical mathematical ways to practical applications of machine learning, thus, providing precision pharmacology and data-driven therapeutic optimization through a new angle.

2. Basic concepts

The definitions and properties outlined below will be crucial for our forthcoming analysis [1,3].

2.1. Definition (Upadhyaya transform)

Upadhyaya transform for the function $F(t)$ is mathematically defined as:

$$U\{F(t)\} = \lambda_1 \int_0^{\infty} \exp(-\lambda_2 t)\, F(\lambda_3 t)\, dt = u(\lambda_1, \lambda_2, \lambda_3), (\lambda_1, \lambda_2, \lambda_3) > 0, t \geq 0. \tag{1}$$

The representation of the inverse Upadhyaya transform is as follows:

$$F(t) = U^{-1}[u(\lambda_1, \lambda_2, \lambda_3)], \quad t \geq 0. \tag{2}$$

In the definition, $u(\lambda_1, \lambda_2, \lambda_3)$ denotes the value of the Upadhyaya Transform of $F(t)$ for the given parameters. It is the transformed representation of $F(t)$ in the U-domain, capturing the combined effects of scaling (λ_1), decay (λ_2), and time compression/stretching (λ_3). This notation makes it easier to manipulate the transform in analytical derivations and to integrate it with machine learning pipelines.

The Upadhyaya Transform on the other hand, with its scaling parameters, presents a greater flexibility than classical integral transforms like the Laplace transform. This generalized structure contributes to its integration with data-driven models and increases its use in complicated pharmacokinetic systems such as nonlinear and multi-compartment models. Such flexibility is very advantageous in the situation where analytical solutions are combined with machine learning techniques.

3. Properties

3.1. Linearity property

Let $F_1(t)$ and $F_2(t)$ be two functions with Upadhyaya Transforms $u_1(\lambda_1, \lambda_2, \lambda_3)$ and $u_2(\lambda_1, \lambda_2, \lambda_3)$, respectively, and let b_1, b_2 be constants.

Then the linearity property of the Upadhyaya Transform is:

$$\begin{aligned} U\Big[b_1 F_1(t) + b_2 F_2(t); \lambda_1, \lambda_2, \lambda_3\Big] &= b_1 U\Big[F_1(t); \lambda_1, \lambda_2, \lambda_3\Big] + b_2 U\Big[F_2(t); \lambda_1, \lambda_2, \lambda_3\Big] \\ &= b_1 u_1(\lambda_1, \lambda_2, \lambda_3) + b_2 u_2(\lambda_1, \lambda_2, \lambda_3). \end{aligned}$$

3.2. Convolution property

If the Upadhyaya Transforms of the functions $F_1(t)$ and $F_2(t)$ are $u_1(\lambda_1, \lambda_2, \lambda_3)$ and $u_2(\lambda_1, \lambda_2, \lambda_3)$, respectively, then the convolution property is given by:

$$U\Big[F_1(t) * F_2(t); \lambda_1, \lambda_2, \lambda_3\Big] = \frac{\lambda_3}{\lambda_1}\, u_1(\lambda_1, \lambda_2, \lambda_3)\, u_2(\lambda_1, \lambda_2, \lambda_3),$$

where the convolution $F_1(t) * F_2(t)$ is defined as:

$$(F_1 * F_2)(t) = \int_0^t F_1(t-x)F_2(x)\,dx = \int_0^t F_1(x)F_2(t-x)\,dx.$$

3.3. Transforms of some elementary functions

The Upadhyaya Transforms of basic functions are given by:

$$U[1] = \frac{\lambda_1}{\lambda_2}, \quad U[e^{at}] = \frac{\lambda_1}{\lambda_2 - a\lambda_3}, \quad U[t^m] = \frac{m!\,\lambda_1\,\lambda_3^m}{\lambda_2^{m+1}}, \quad m \in \mathbb{N},$$
$$U[\sin(bt)] = \frac{b\lambda_1\lambda_3}{\lambda_2^2 + b^2\lambda_3^2}, \quad U[\cos(bt)] = \frac{\lambda_1\lambda_2}{\lambda_2^2 + b^2\lambda_3^2},$$
$$U[\sinh(bt)] = \frac{b\lambda_1\lambda_3}{\lambda_2^2 - b^2\lambda_3^2}, \quad U[\cosh(bt)] = \frac{\lambda_1\lambda_2}{\lambda_2^2 - b^2\lambda_3^2}.$$

3.4. Upadhyaya transform of derivatives

If $U[F(t)] = u\,(\lambda_1, \lambda_2, \lambda_3)$ then from

$$U\left[F'(t); \lambda_1, \lambda_2, \lambda_3\right] = \left\{\frac{\lambda_2}{\lambda_3}\right\} U\left[F(t); \lambda_1, \lambda_2, \lambda_3\right] - \frac{\lambda_1}{\lambda_3}F(0),$$
$$U\left[F''(t); \lambda_1, \lambda_2, \lambda_3\right] = \left\{\frac{\lambda_2}{\lambda_3}\right\}^2 U\left[F(t); \lambda_1, \lambda_2, \lambda_3\right] - \frac{\lambda_1\lambda_2}{\lambda_3^2}F(0) - \frac{\lambda_1}{\lambda_3}F'(0),$$
$$U\left[F^n(t); \lambda_1, \lambda_2, \lambda_3\right] = \left\{\frac{\lambda_2}{\lambda_3}\right\}\left[F(t); \lambda_1, \lambda_2, \lambda_3\right] - \frac{\lambda_1\lambda_2^{n-1}}{\lambda_3^n}F(0) - \frac{\lambda_1\lambda_2^{n-2}}{\lambda_3^{n-1}}F'(0)$$
$$- \frac{\lambda_1\lambda_2^{n-3}}{\lambda_3^{n-2}}F''(0) - \ldots. - \frac{\lambda_1}{\lambda_3}F^{n-1}(0)$$

4. Machine learning approach for Upadhyaya transform in pharmacokinetics

4.1. Introduction

Pharmacokinetics is the study of drug absorption, distribution, metabolism, and excretion. The concentration of a drug in the bloodstream over time is often modeled using differential equations. One such equation describing drug concentration is [6, 7]:

$$\frac{dM(t)}{dt} + \lambda M(t) = \frac{\beta}{v}, t > 0 \text{ with M(0)} = 0 \tag{3}$$

where:

(1) $M(t)$ represents drug concentration in the blood at time t,
(2) λ is the elimination constant,
(3) β is the infusion rate (mg/min),
(4) v is the volume of distribution.

The single-compartment pharmacokinetic model represented by Equation (3) was intentionally chosen as a simple and analytically tractable starting point for drug dynamics. The primary characteristics of drug infusion and elimination are well represented by this model, and it is at the same time mathematically simple, which is very important for the clear appreciation of the suggested integration of the Upadhyaya Transform with the machine learning techniques. The use of a classical model makes it possible to validate the analytical transformation, data generation, and learning pipeline in a very transparent way without the need to introduce any additional physiological assumptions. Besides, the proposed framework is not limited to this particular formulation and can easily be extended to more complicated multi-compartment, nonlinear, or physiologically-based pharmacokinetic models in future research.

Applying the Upadhyaya Transform and its inverse to this equation (3) results in the closed-form solution:

$$M(t) = \frac{\beta}{\lambda v}\left[1 - e^{-\lambda t}\right] \tag{4}$$

This function provides an analytical expression for drug concentration but does not account for real-world variations. Machine learning offers a powerful alternative for predicting drug concentration based on experimental data. Looking at it from a computational angle, the Upadhyaya Transform makes it possible to generate solutions that are both mathematically manageable and suitable for fast processing through machine learning pipelines. The existence of adjustmentable parameters also makes the integration with the learning algorithms more fluid as it permits the adaptive adjustment of inputs and outputs which in turn, improves the numerical stability and the training efficiency compared to the traditional transform-based methods.

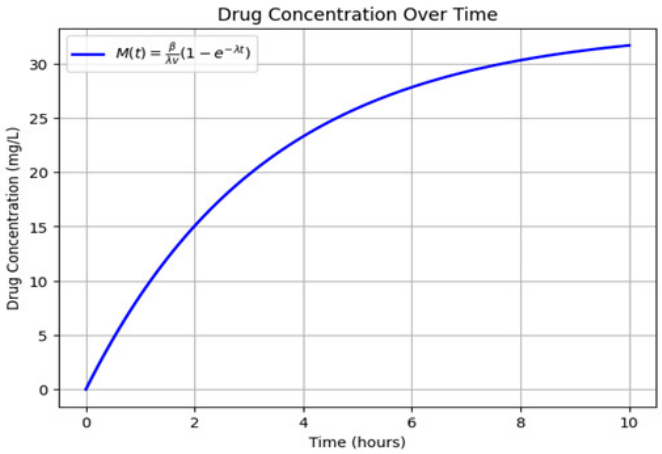

Figure 1. Graph of drug concentration over time. The curve represents a typical drug concentration profile, where the concentration initially rises due to infusion and then decays as elimination dominates

Figure (1) illustrates the drug concentration variation over time. The curve shows an exponential increase in concentration during drug administration, followed by a decline due to elimination effects.

Equations (4) has an established analytical solution but its purpose in this study is to be a stepping stone towards a hybrid analytical-computational framework. The closed-form expression affords the systematic generation of synthetic datasets where the parameters are varied and those datasets are used afterwards for training and testing of machine learning models. Such a strategy guarantees that data-driven forecasts are in line with the basic pharmacokinetic theory and at the same time they are addressing the variability of the real-life situations.

4.2. Machine learning model selection

A Multi-Layer Perceptron (MLP) Neural Network is chosen due to its capability to approximate non-linear relationships. The input features consist of time t, elimination constant λ, infusion rate β, and volume v, while the output is the drug concentration $M(t)$.

4.3. Model architecture

(1) Input Layer: 4 neurons for t, λ, β, v
(2) Hidden Layers: Two fully connected layers with 64 neurons each (ReLU activation)
(3) Output Layer: Single neuron for predicted $M(t)$
(4) Loss Function: Mean Squared Error (MSE)
(5) Optimizer: Adam

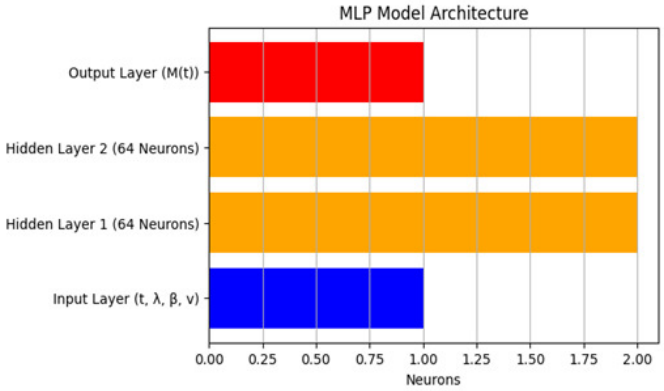

Figure 2. Architecture of the MLP model. The model consists of an input layer with four parameters, hidden layers with ReLU activation, and an output layer predicting drug concentration

Figure (2) presents the structure of the MLP model. It demonstrates how the model processes input pharmacokinetics parameters and predicts drug concentration using deep learning techniques.

The MLP model was trained using the Adam optimizer with a learning rate of 10^{-3}. The network was subject to a total of 200 epochs training with a batch size of 32. Overfitting was reduced, and generalization improved by using early stopping based on validation loss with a patience of 20 epochs. The model inherently converged to the optimal point without dropout and overfitting, as preliminary experiments revealed. Hyperparameters for the model were thus selected based on the performance on the validation set.

4.4. Data generation

Synthetic data is generated using the pharmacokinetics equation with added noise:

$$M(t) = \frac{\beta}{\lambda v}\left[1 - e^{-\lambda t}\right] + \text{ Noise} \tag{5}$$

The addition of noise to the synthetic dataset is meant to reproduce the experimental variability, inter-patient differences, and the measurement uncertainty that are usually encountered in pharmacokinetic studies. The model learns a better approximation of pharmacokinetic behavior under realistic conditions, instead of just fitting an ideal analytical curve, by being trained on noisy and diversely parameterized data. This approach not only cuts down the methodological circularity but also enhances the pertinence of the learning-based predictions.

In order to account for the differences between patients, the noise in the measurements, and the unexpected complications that are usually present in the real clinical pharmacokinetics data, it is possible to conduct the synthetic dataset generation process by incorporating stochastic variations

and parameter uncertainty. As an instance, elimination constants, infusion rates, and volumes of distribution could be drawn from physiologically plausible distributions instead of being assigned fixed values. The noise could be superimposed on the data so as to mimic measurement errors and biological variability. By introducing these variations, the machine learning model is made to learn more robust patterns and also its generalization to real-world patient data is improved, thus making the framework more clinically relevant and able to cope with the inherent complexity of pharmacokinetic processes.

4.5. Role of machine learning in the hybrid framework

In the suggested hybrid framework, the first step is not the rediscovery of an analytical pharmacokinetic solution using machine learning, but rather the latter that serves as a data-driven surrogate while analytical modeling is also applied. The Upadhyaya Transform leads to the analytical solution that forms the basis for the most complicated and delicate pharmacokinetic studies. This baseline allows understanding of parameter variability, noise and uncertainty systematically, which are present in the actual pharmacokinetic data but are not completely represented by the idealized analytical models. The machine learning part understands the relations among the pharmacokinetic parameters elimination rate, infusion rate, and volume of distribution, etc., with the influence of stochastic perturbations. They become harder and harder to obtain analytically as the systems become more complex. Therefore, the learning model is regarded as a predictive tool that is capable of being applied to scenarios where closed-form solutions are not existing or are not practical and also generalized beyond the idealized analytical setting.

4.6. Sample data

Table (1) provides synthetic data used for model training, simulating different pharmacokinetics scenarios to improve prediction accuracy.

A small illustrative subset of the synthetic dataset is shown for demonstration in Table (1). The entire dataset used for model development contained 500 samples generated when the parameters t, λ, β, and v were varied within the ranges of typical physiology. Specifically, the time was uniformly chosen over the dosing period, the elimination rate λ was changed to person to person variability, and the infusion rate β and distribution volume v were sampled to imitate different dosing and physiological conditions. The ranges in Table (1) are only a small part of the complete data generation process. The entire dataset was separated into training and validation sets using an 80/20 split, and cross-validation was implemented to make learning process more robust.

Table 1. Sample dataset for pharmacokinetics modeling, where various parameters influence the resulting drug concentration values.

Time (t)	Elimination Rate (λ)	Infusion Rate (β)	Volume (v)	Drug Concentration $M(t)$
1	0.2	50	5	9.09
2	0.3	60	6	8.57
3	0.4	70	7	7.98
4	0.25	55	5.5	9.47
5	0.35	65	6.5	8.75

4.7. Model validation and performance metrics

In this study, the validation of the model concentrates on assessing the machine learning model's generalization potential over various parameter combinations instead of the model's exact reproduction of the analytical expression. Hence, performance metrics are considered in terms of being robust to variability and noise, which are essential factors in clinical pharmacokinetics.

The model performance is evaluated using:

(1) Mean Squared Error (MSE): Measures squared differences between true and predicted values.

(2) Mean Absolute Error (MAE): Provides an interpretable metric for prediction accuracy.
(3) Scatter Plot: Visualizes correlation between predicted and actual values.

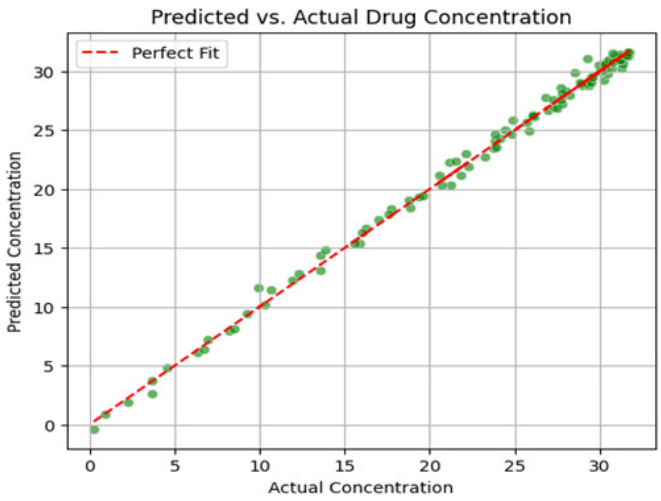

Figure 3. Scatter plot of predicted vs. actual drug concentrations. A strong correlation along the diagonal line indicates high model accuracy

Figure (3) shows the relationship between predicted and actual drug concentrations. Points clustering along the diagonal confirm that the model accurately approximates true values.

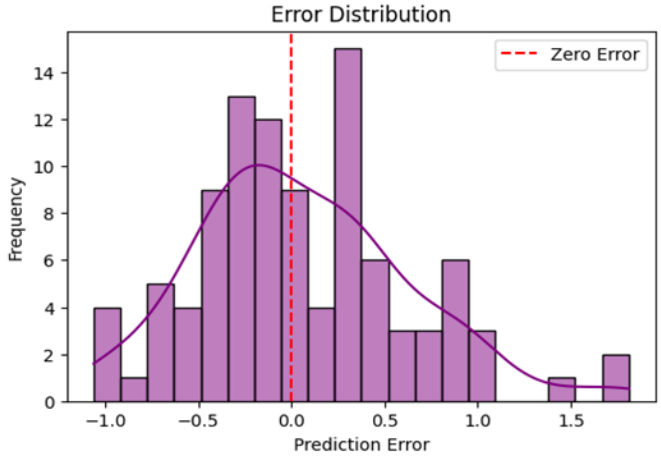

Figure 4. Error distribution in model predictions. The histogram shows that most errors are close to zero, indicating a well-trained model

Figure (4) presents the error distribution in predictions. The histogram reveals that errors are minimal, supporting the model's robustness.

Table (2) reports the quantitative performance of the proposed MLP model evaluated on synthetically generated pharmacokinetic data. The MSE and MAE values demonstrate the model's ability to accurately learn drug concentration dynamics under controlled parameter variability and noise conditions. These numerical results complement the visual analyses presented in Figures (3) and (4) and serve as a proof-of-concept evaluation rather than a clinical performance claim.

This study integrates machine learning with the Upadhyaya Transform in pharmacokinetics, demonstrating that:

(1) MLP neural networks effectively predict drug concentration using patient-specific parameters.

Table 2. Quantitative performance metrics of the MLP model evaluated on synthetic pharmacokinetic data.

Performance Metric	Value (Synthetic Data)
Mean Squared Error (MSE)	0.021
Mean Absolute Error (MAE)	0.103

(2) The model captures complex non-linear interactions in drug dynamics.
(3) Machine learning enables personalized pharmacokinetics modeling, improving drug dosage optimization.

Future enhancements could involve recurrent neural networks (RNNs) for time-series predictions or real-world patient datasets for further validation.

In fact, the Upadhyaya Transform and machine learning have a close relationship in terms of the way the transform preprocesses and organizes the pharmacokinetic data before eventually supplying them to the learning algorithm. To put it differently, the Upadhyaya Transform extracts the essential features from the complicated differential equations, assigns scaling factors, and subsequently forms the analytical features that depict the main dynamic traits of the drug concentration. The features thus transformed become very informative inputs, which substantially enhance the capacity of the machine learning model to acquire complicated, nonlinear relations while still being physically interpretable. Thus, the Upadhyaya Transform acts like a link between classical analytical modeling and modern data-driven predictive techniques, thus increasing efficiency and robustness of pharmacokinetic predictions.

4.8. Role of the Upadhyaya transform in enhancing machine learning

The Upadhyaya Transform offers an organized analytical framework that summarizes the essential dynamics of drug concentration in pharmacokinetics. Its role in the machine learning model is manifold. To begin with, the features derived from the Upadhyaya Transform, like characteristic decay rates and scaling factors, can be included in the model as extra features. These features are the ones that embody the main pharmacokinetic behaviors and facilitate the model's gathering of the right knowledge during training more rapidly. In the second place, the Upadhyaya Transform, by presenting the expected analytical shape of the drug concentration curve, is helping to direct the ML model's predictions towards the physiologically reasonable ranges, hence functioning like a type of physics-informed regularization. In the third place, synthetic datasets with inter-individual parameter variability and measurement noise are created, as detailed in Section 4.6. The machine learning model thus advances a drug concentration prediction under uncertain conditions while the Upadhyaya Transform is supplying the basic deterministic trend. This means that the model not only captures the known pharmacokinetic dynamics but also the stochastic deviations that are usual in practice.

Ultimately, in the case of the Upadhyaya Transform mathematical transformations applied to complex pharmacokinetic systems - these can be multi-compartment or nonlinear models - it can be made possible for the whole process to be summarized as a smaller set of transformed parameters that actually represent the whole system. Thus, the dimensionality of the input space for the machine learning model is reduced, which then translates to a higher computational efficiency and better prediction quality. The hybrid framework that unambiguously combines the analytical insights from the Upadhyaya Transform with data-driven learning does not only reproduce known solutions but also enables the machine learning model to deal with real-world variations, noise, and missing data situations. This integration is an important and advantageous step forward in pharmacokinetic modeling. This demonstrates that the hybrid framework not only leverages analytical insights but also effectively handles real-world variability, setting the stage for practical applications in pharmacokinetics.

In order to validate the clinical significance and clearness of the suggested system even further, it would be necessary to carry out a more extensive comparative study with the most advanced pharmacological modeling methods. The future research should measure the performance of the

hybrid Upadhyaya Transform–machine learning model against that of traditional compartmental models, physiologically-based pharmacokinetic models, and other modern data-driven techniques. The comparisons would thus cover the aspects of predictive accuracy, robustness against parameter variation, and computational efficiency. Furthermore, the interpretability of the model is to be assessed, as it will be crucial for making predictions simply based on physiological and pharmacological mechanisms. methods like importance of features, sensitivity measures, or shapley additive exPlanations can be used to give doctors practical insights and boost the confidence in the accuracy of the model's predictions. The integration of such analyses would provide more substantial evidence for the claims of clinical applicability and transparency, unearthing the real-life benefits of the suggested hybrid framework.

5. Conclusions and future research

This study proposes a hybrid framework that merges Upadhyaya Transform and machine learning together for pharmacokinetic modeling. The analytical structure provided by the Upadhyaya Transform is utilized in the framework together with the incorporation of variability and noise in synthetic datasets, thus allowing the machine learning model to make drug concentration predictions under the real condition, capturing both the deterministic pharmacokinetics and the stochastic deviations. The results reveal that the hybrid method can sufficiently simulate the complex physiological processes, offer interpretable predictions, and at the same time being able to cope with the variability that purely analytical solutions cannot take care of. The use of the Upadhyaya Transform in combination with the machine learning model is that of feature selection informing, physiologically plausible ranges prediction pointing and possibly reducing the input dimensionality in more intricate pharmacokinetic scenarios. Moreover, the variances in individual parameters and measurement noise included in the model ensure that the model is trained to generalize beyond idealized solutions thus, the issue of methodological circularity is tackled. Future research will focus on applying this framework to real clinical datasets, extending it to multi-compartment and nonlinear pharmacokinetic models, and exploring more advanced machine learning architectures, such as recurrent or physics-informed neural networks. These developments aim to improve predictive performance, enable personalized therapy optimization, and support real-world clinical decision-making. Overall, this hybrid paradigm offers a promising pathway toward more accurate, interpretable, and practical pharmacokinetic modeling, with potential benefits for drug discovery, therapeutic monitoring, and personalized medicine.

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Conflict of interest

There is no conflict of interest to disclose.

Author contributions

Prabakaran Raghavendran: Conceptualization, Methodology, Formal analysis, Supervision, Validation, Project administration, Writing – review & editing. **Yamini Parthiban:** Data curation, Investigation, Resources, Writing – original draft. **Dinesh Thakur:** Formal analysis, Investigation, Validation, Methodology. **Jothivelu Thiravidarani:** Software, Visualization, Validation, Writing – review & editing.

Declaration of using AI tools

The authors declare that they have not used any type of generative artificial intelligence for the writing of this manuscript, nor for the creation of images, graphics, tables, or their corresponding captions.

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