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Analysis of Drug Absorption Rate Using Fuzzy Matrices, PCA, and Machine Learning

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KEYWORDS:

Matrices, PCA, and Machine Learning

ABSTRACT:
The present study mainly focuses on calculating drug absorption in the human body by considering key physiological parameters namely gastric pH, metabolic rate, and partition coefficient. It is difficult to predict the medication absorption in human body accurately due to factors like biological uncertainty and inter- individual variability, to overcome this problem A hybrid model strategy is used which combines fuzzy theory, machine learning, and statistical analysis. The main input factors of the models are Gastric pH, metabolic rate, and partition coefficient. To lower the complexity of the data set the most important parameters are found using Principal Component Analysis (PCA), and to estimate and reduce the prediction errors, statistical techniques are used. And lastly optimization techniques are used to identify circumstances that enable more effective and regulated drug absorption.

Introduction:

Due to many physical and biochemical factors the drug absorption becomes a complex problem, It often vary from person to person and involve uncertainty. Initially pharmacokinetic models were usually used which have fixed parameters and simple assumptions which not always able to capture this fluctuations accurately that makes the task of predicting drug absorption difficult. To overcome this limitations, now days advanced computational methods are used by many researchers this methods learn from data and handle uncertainty effectively. In this regard hybrid modeling approaches are useful as the combine the strengths of different techniques.

In the present study, a hybrid model is proposed that combines fuzzy logic, Principal Component Analysis (PCA), and machine learning to improve the prediction of drug absorption. Unlike traditional methods, this approach can handle uncertainty using fuzzy logic, reduce the number of variables using PCA for better understanding, and use machine learning to make accurate predictions within a single framework.

The main objectives of this study are: (i) to represent uncertain pharmacokinetic parameters using fuzzy logic, (ii) to apply PCA to reduce features and identify important factors, and (iii) to train machine learning models to effectively predict the drug absorption rate.

2. Literature Review and Research Gap

In the earlier studies of medication absorption the main tools were Regression based or compartmental pharmacokinetic models, these models are generally used for well controlled parameters, but they are not adaptable to unpredictable biological situations. Recent research used PCA for feature reduction in bioinformatics and fuzzy systems for medical diagnosis. Researcher are also succesfully using machine learning techniques like Random Forests and Support Vector Machines for Pharmacological predictions. Few research have also combines fuzzy logic, PCA, and ML into a unified drug absorption modeling. This hybridization fixes three critical limitations:

1. Managing uncertainty
2. Dimensionality reduction
3. and comprehensibility.

Therefore the goal of this research is to incorporate hybrid system that connects computer prediction models with traditional pharmacokinetics.

3. Methodology

The proposed framework consists of three integrated modules: Fuzzification, Principal Component Analysis (PCA), and Machine Learning.

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3.1 Fuzzification

To convert important physiological and biochemical parameters, such as gastric pH, partition coefficient (log P), enzyme activity, blood pressure, cholesterol, and blood cell levels into fuzzy sets, Triangular and trapezoidal membership functions were used. This step helps in handling uncertainty present in the data and also brings all the input values to a common scale, making them suitable for further analysis.

Data Matrix Example:

$$X = \begin{matrix} \\ PH \\ Log\ P \\ Enzy.\ Act. \end{matrix} \begin{matrix} \text{Low} & \text{Medium} & \text{High} \\ \end{matrix} \begin{bmatrix} 2 & 5 & 7 \\ 0 & 3 & 4 \\ 0.2 & 0.5 & 0.9 \end{bmatrix}$$

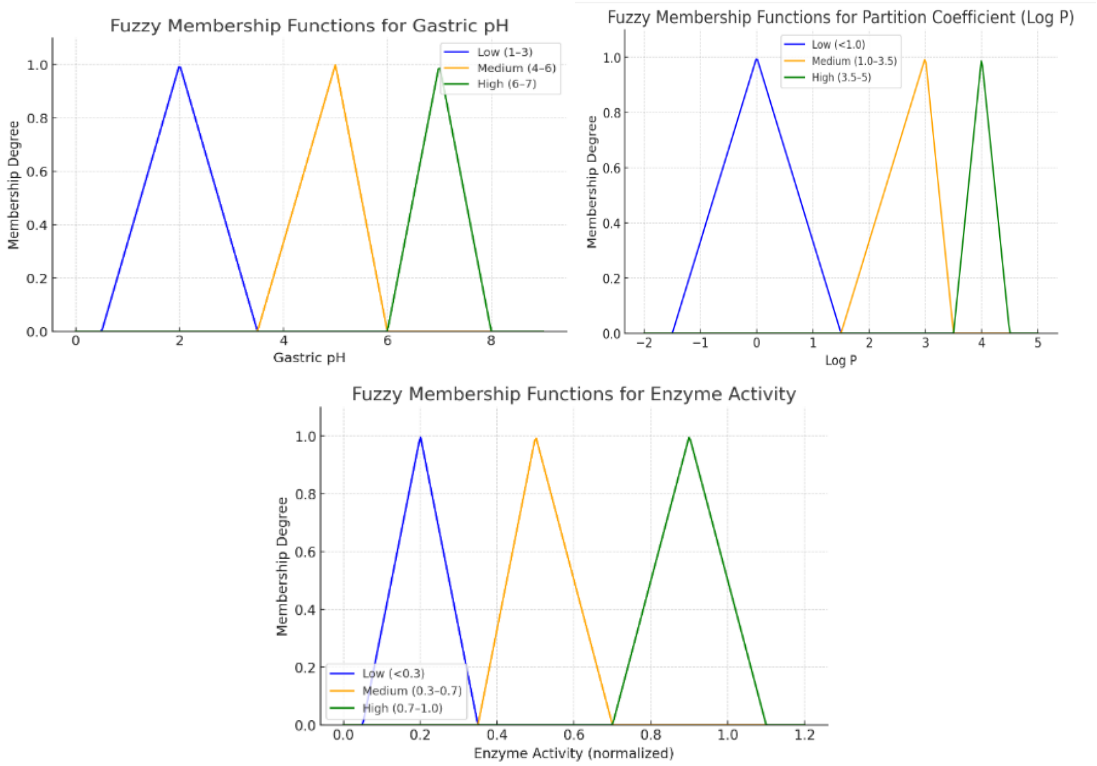
Using Triangular membership function:

$$\mu(x;a,b,c) = \begin{cases} 0 & ,x \le a \\ \dfrac{x-a}{b-a}, & a < x \le b \\ \dfrac{c-x}{c-b}, & b < x < c \end{cases}$$

then Fuzzified (normalized) matrix is given by:

$$\mu(X) = \begin{matrix} \\ PH \\ Log\ P \\ Enzy.\ Act. \end{matrix} \begin{matrix} \text{low} & \text{med} & \text{high.} \\ \end{matrix} \begin{bmatrix} 1.0 & 0 & 0 \\ 1 & 1.0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Figure 1: Graphical representation of Fuzzy degree



3.2 Principal Component Analysis (PCA)

To preserve much of the variance while reducing dimensionality the fuzzified dataset was subjected to PCA. To identify principal components Covariance and eigen decomposition were performed. In order to highlight the most significant elements influencing absorption rate variability, the top two components were chosen for feature modification.

Mean Calculation

PH = 0.333333, LogP = 0.666667, Enzy.Act. = 0.333333.

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Centered matrix of Data: difference of mean and elements of $\mu(X)$

low medium high

$$Zcen = \begin{matrix} PH \\ Log\ P \\ Enz.Act \end{matrix} \begin{bmatrix} 0.66 & -0.33 & -0.33 \\ 0.33 & 0.33 & -0.66 \\ -0.33 & -0.33 & 0.66 \end{bmatrix}$$

Covariance Matrix:

$Cov(F) = \frac{1}{n-1} {Z_{cent}}^T Z$ *take n=3 we get 3by 3 matrix*

$$C = \begin{bmatrix} 0.33 & 0.16 & -0.16 \\ 0.16 & 0.33 & -0.33 \\ -0.16 & -0.33 & 0.33 \end{bmatrix}$$

Eigen Values are

λ_1 =0.788, λ_2 = 0.211, $\lambda_3 = 0$ (take only two higher values) numerically approximate

Unit eigen vectors corresponding to eigen values:

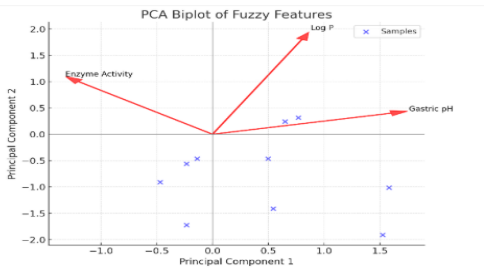
$$e_1 = \frac{X11}{\|X11\|} = \begin{bmatrix} 0.4082 \\ 0.8165 \\ -0.4082 \end{bmatrix}, e_2 = \frac{X12}{\|X12\|} = \begin{bmatrix} 0.4082 \\ -0.4082 \\ 0.8165 \end{bmatrix}$$

For PC1 and PC2: **Principal Component Selection and Projection** Retain top 2 components:

$Y = {e_i}^T component\ of\ Z_{cent}$

Features	*PC1*	*PC2*
Low	0.6736	−0.1347
Medium	0.2694	−0.5389
High	−0.9435	0.6736

Figure 3: PCA biplot showing projected samples and eigenvector directions for the four fuzzy features:



What this means for drug absorption?

Good absorption efficiency, balanced PC2, and high PC1. The main factor influencing absorption rate variation is PH, Log P has a significant projection on PC1 and PC2, and enzyme activity adds to variance that is positively aligned with Log P but opposed to PC1 for PH.

3.3 Machine Learning Integration

To trained the models like Random Forest Regressor and Support Vector Machine, the simplified data so obtained from PCA is used. and to check how well these models work, Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), and coefficient of determination (R2) were used. These measures helps us to understand how accurate and reliable the predictions of the model are.

Performance Metrics:

Actual Value (y)	Predicted Value ($\bar{y}$)
0.60	0.75
0.80	0.85
0.90	0.98

$MAE = \frac{\Sigma|y_i - \hat{y}|}{n} = 0.093$

It interpret average magnitude of errors in a set of predictions it is given by absolute difference of actual and predicted values. Obtained value 0.093 units represents rate of absorption differ to target variable by this value.

$RMSE = \sqrt{\frac{\Sigma(y_i - \hat{y})^2}{n}} = 0.1023$

Root mean square error (RMSE) interpreted as the average prediction error, in the same units as the drug absorption rate.

$R^2 = 1 - \frac{\Sigma(y_i - \hat{y})^2}{\Sigma(y_i - \bar{y})^2}, = 0.3271$, where $\bar{y}$ is the mean of actual values.

R squared value measures the proportion of the variance in the dependent variable (drug absorption rate) that is predictable from the independent variables (features).

Figure 4: Actual vs Predicted Drug Absorption Rate

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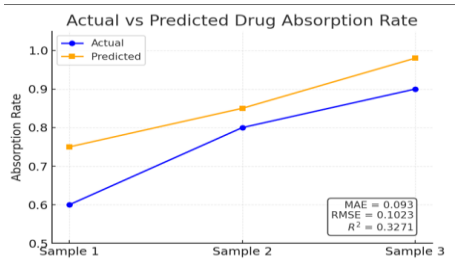

4. Result and Discussion

This study is a hybrid model which improve the

In this Study, the hybrid model helped to improve the stability of predictions. The R^2 values showed that the model fits the data well, while the low MAE and RMSE values indicate that the difference between actual and predicted drug absorption is small. Compared to existing pharmacokinetic and machine learning methods, the proposed fuzzy–PCA–ML model handles uncertainty better and is easier to interpret.Additionally, a comparison between oral and intraperitoneal drug delivery was included, which showed differences in absorption efficiency, without going into clinical details.

All figures and tables in the paper are clearly numbered, properly labeled, and correctly referred to in the text. For example, the PCA biplot and model performance graphs include appropriate titles and legends for better understanding.

5. Conclusion and Applications:

It is a new hybrid model which is a combination of fuzzy logic, PCA, and machine learning to predict accuracy of drug absorption. The model improves prediction by handling uncertainty, reducing unnecessary data, and making the results easier to understand. It provides a more reliable computational approach for studying drug absorption.

The model can also be useful in personalized medicine, as it supports data-based dose optimization and may reduce the need for extensive experimental trials. In the future, the model can be further improved by including real-time patient data and testing it on clinical datasets to make it more practical and applicable in real-world situations.

Applications

1. This can reduce trial and error in clinical testing, making drug development faster and less costly.

2. This work can help pharmaceutical researchers choose **optimal delivery routes** for medications.

3. **Dosages can be fine-tuned** to avoid side effects or under-dosing. This is especially important for **critical drugs** like antibiotics, cancer therapies, or pain medications.

4. This approach can be adapted to **individual patient data** (age, weight, metabolism, enzyme activity) to customize drug doses also helps to ensure patients receive **the right drug at the right dose**, improving treatment success.

5. This paper shows how computational models can **complement lab experiments**.

6.. This improves **drug safety regulations** and ensures **cost-effective healthcare solutions**

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