Metaheuristics Applied to Optimal Feature Selection for Accurate Predictive Models in Smart Health: A Case Study on Hypotension Prediction in Hemodialysis Patients

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Abstract: Predicting potential hypotensive episodes in chronic kidney disease patients before dialysis is crucial for preventing complications and ensuring effective treatment. This study explores the use of metaheuristic algorithms to optimize the complex task of selecting the feature set needed to develop a highly accurate predictive machine learning model for detecting hypotension, based on clinical parameters from the dialyzer and analytical data from blood tests. Metaheuristic algorithms offer a robust approach to optimal variable selection and subsequent dimensionality reduction, leading to more accurate machine learning predictor models. In this context, two relevant metaheuristic algorithms were employed: Particle Swarm Optimization (PSO) and Grey Wolf Optimizer (GWO), along with the supervised machine learning algorithm XGBoost. The results demonstrate that the application of metaheuristic techniques not only reduces the feature count from 67 to 36 variables but also improves classifier performance, thereby enhancing the prediction of hypotensive events. Specifically, the optimized model achieved an Area Under the Curve (AUC) of 0.76 and a recall of 0.764 for the minority class (hypotensive episodes) in chronic kidney disease patients prior to hemodialysis procedures.

1 INTRODUCTION

1.1 The Challenge of Early Detection of Intradialytic Hypotension

Dialysis and transplantation have allowed many patients with advanced chronic kidney disease (CKD) to live longer and maintain a good quality of life. Over the last decade, the prevalence of advanced CKD has increased by nearly 30% in Spain. As a result, in 2021, 65,740 patients required dialysis to stay alive, with 26,690 of them undergoing hemodialysis (HD) techniques (Sociedad Española de Nefrología, 2023).

Intradialytic hypotension (IDH) is one of the most common adverse events during hemodialysis (HD) sessions. Despite significant advances in HD techniques in recent decades that have improved its management, IDH remains prevalent, occurring in 5-40% of sessions (Flythe et al., 2020). This condition is associated with high morbidity and mortality rates, as well as multiple complications. Currently, there are no standardized guidelines or systematic treatments for managing IDH; various maneuvers are employed to control it (Furaz Czerpak et al., 2014). IDH is char-

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acterized by three essential components: a drop of more than 20 mmHg in systolic blood pressure (SBP) or more than 10 mmHg in mean arterial pressure (MAP), the presence of ischemic symptoms in various organs, and interventions by dialysis staff (Agarwal, 2012).

Identifying the occurrence of intradialytic hypotension (IDH) during hemodialysis (HD) treatment is challenging due to the numerous variables involved, including the type of dialyzer, dialyzer temperature, patient characteristics, dialysis modality, and medical criteria. Therefore, pinpointing the factors that most significantly influence the occurrence of IDH and predicting its onset would provide valuable decision support for medical staff.

1.2 Prediction of IDH Using Machine Learning Techniques

Determining whether a patient experiences intradialytic hypotension (IDH) during hemodialysis (HD) treatment is a complex task for traditional statistical models. However, machine learning (ML) models can effectively discover patterns in the data, making them particularly well-suited for this problem (Nayyar et al., 2021). This work aims to identify an optimal ML-based model to predict the likelihood of IDH at the start of HD treatment. To achieve this, metaheuristic techniques will be employed to select the best combination of variables from the patient's clinical and analytical blood records, which contain numerous characteristics, to reduce noise, improve model performance, and enhance the accuracy of the ML model.

Recent research has developed predictive models that utilize machine learning algorithms and optimization techniques to forecast intradialytic hypotension (IDH) episodes with high accuracy. These models empower healthcare professionals to anticipate and prevent IDH, thereby enhancing patient safety and well-being during hemodialysis treatments. By combining machine learning with optimization techniques, significant progress has been made in managing and preventing health complications. Various studies have proposed different methodologies to predict and manage IDH episodes, aiming to improve patient outcomes and enhance clinical decision-making. For instance, Hong et al. (Hong et al., 2023) introduced a software-based artificial intelligence alert system to identify patients at high risk of IDH before hemodialysis sessions. Similarly, Gervasoni et al. (Gervasoni et al., 2023) developed and validated two AI-based risk models to predict symptomatic IDH at different time points. Othman et al. (Othman et al., 2022) focused on early alert systems, employing AI and machine learning techniques for IDH prediction prior to the initiation of hemodialysis. In another approach, Yang et al. (Yang et al., 2022) presented a hybrid model, BSCWJAYA-KELM, which integrates serum biomarkers with a novel optimization algorithm to enhance prediction accuracy. Additionally, Chen et al. (Chen et al., 2020) investigated clinical factors associated with IDH using deep learning, while Lee et al. (Lee et al., 2023) developed a model based on pre-dialysis features for IDH prediction. Zhang et al. (Zhang et al., 2023) utilized a machine learning model to predict IDH in in-center hemodialysis patients 15 to 75 minutes in advance. Kim et al. (Kim et al., 2022) introduced a deep learning model that relies solely on monitoring measurements from hemodialysis machines, and Mendoza-Pittí et al. (Mendoza-Pittí et al., 2022) created a machine learning model capable of predicting IDH at the start of hemodialysis sessions. Finally, Gómez-Pulido et al. (Gómez-Pulido et al., 2021) predicted hypotension using models trained on a large dialysis database.

These studies collectively enhance the understanding of intradialytic hypotension (IDH) prediction and management through the use of machine learning algorithms and AI techniques. Their aim is to identify high-risk patients early, facilitating timely interventions to prevent acute hypotension during hemodialysis and ultimately improving patient outcomes.

1.3 Optimal Feature Selection Technique Based on Metaheuristics

In the healthcare field, innovative and efficient solutions to complex problems are crucial (Haupt and Haupt, 2004). Metaheuristics, which include algorithms such as genetic algorithms, particle swarm optimization, and ant colony optimization, have significant applications in this sector. These algorithms iteratively search for optimal solutions by initializing a population of candidate solutions and evaluating their fitness according to an objective function. Based on this evaluation, they generate new populations by modifying the existing ones to enhance overall fitness. This process, illustrated in Fig. 1, continues until a stopping criterion is met.

These techniques are employed to optimize medical treatments, enhance hospital scheduling, and facilitate the analysis of large medical datasets. The ability of metaheuristics to identify near-optimal solutions within a reasonable time frame makes them ideal for addressing healthcare challenges, where swift and accurate decisions can significantly impact patient outcomes (Rahul and Banyal, 2022; Aljohani, 2024).

The Feature Selection (FS) problem is a multi-objective combinatorial optimization challenge that arises from the need to eliminate irrelevant and redundant information from datasets used in machine learning training. Such irrelevant information can hinder the performance of prediction or classification algorithms.

In its mathematics definition, FS assumes a dataset O such as the original dataset, which contains a o number of f features, such that $O = \{f_1, f_2, f_3, \ldots, f_o\}$. The objective of the problem is to select the best subset of features $B = \{f_1, f_2, f_3, \ldots, f_b\}$ with $b < o$ so that the features belonging to the selected subset are the most representative of the set of original data. (Ebiaredoh-Mienye et al., 2022; Pudjihartono et al., 2022)

Internally, feature selection operates within a binary domain, where solutions are represented by ones and zeros. A one indicates that a feature is included in the data subset, while a zero signifies its exclusion. Fig. 2 illustrates this representation for the feature selection problem. In this example, the original dataset comprises six features, resulting in the solution $[1,1,1,1,1,1]$. After applying the metaheuristics, the optimal subset of features, which includes features f_1, f_2, and f_3, is identified, yielding the solution $[1,0,1,1,0,0]$.

The objective function to optimize within the feature selection problem is represented in different ways, but the most used is the weighted multi-objective function (Barrera-García et al., 2023). In this way, the objective function Z is calculated as the following equation (1):

$$min\, Z = \alpha \cdot metric + \beta \cdot \frac{|R|}{|N|} \tag{1}$$

where *metric* corresponds to a performance metric obtained from the machine learning technique, $|R|$ is the number of selected features, and $|N|$ the total number of features, with $\alpha \in [0,1]$ and $\beta = (1-\alpha)$ parameters that regulate the importance of the quality of the results and the size of the subset, respectively.

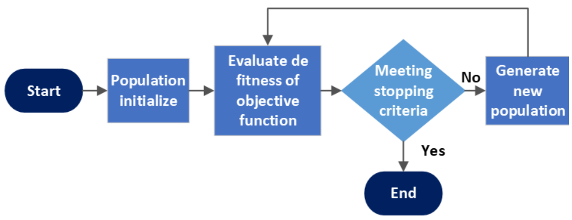

Figure 1: Flowchart of the metaheuristic algorithm process.

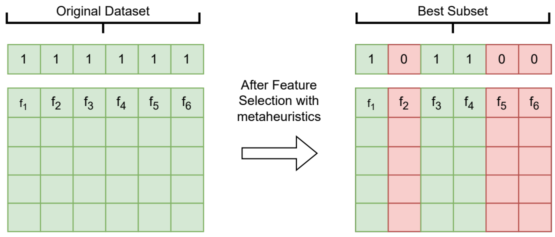

Figure 2: Binary representation of vectors S and D.

1.4 Hypothesis

It is possible to detect an optimal combination of clinical and analytical parameters associated with the development of IDH.

By analyzing a patient's previous analytical values and relevant data, along with measurements of specific clinical parameters at the beginning of a hemodialysis (HD) session, it may be possible to predict the occurrence of an intradialytic hypotension (IDH) episode. This could help reduce its incidence and enable early intervention by medical staff. The research aims to extract and construct a subset of significantly relevant variables from a large database of HD sessions and blood tests. This subset will be suitable for processing with mass data tools and will facilitate the prediction of IDH based on patterns derived from an optimal and reduced set of clinical and analytical parameters.

2 MATERIALS AND METHODS

2.1 Digitized Clinical Database of Hemodialysis Patients

Our research is based on two extensive databases containing medical information from 758 patients undergoing hemodialysis sessions at Hospital Príncipe de Asturias in Madrid, Spain, over nearly four years, from January 1, 2016, to October 30, 2019. The first database includes clinical data for 98,015 hemodialysis sessions, each lasting about five hours, and comprises patient and session identification data along with 180 clinical parameters automatically recorded by the dialyzer during the sessions. The second database contains blood analysis data for the same patients and period, featuring 141 variables arising from routine blood tests performed at varying intervals.

To create the dataset for this study, the two databases were merged such that each hemodialysis session was linked to both the session's clinical data and the results of the blood test closest in time—either on the same date or immediately prior. In total, this merging process resulted in a new dataset containing 221 variables related to patient information, dialysis sessions, and blood tests. The collection of these records was approved by the hospital's ethics committee, with all data fully anonymized.

2.2 Database of HD Sessions Indicating IDH Events

In the integrated database, HD sessions in which the IDH event is determined by medical criteria are marked. For this purpose, it is determined from the systolic arterial pressures measured in each of the 5 hours of the session whether the difference between any of these pressures measured during the session is at least 20 mmHg lower than the pressures measured at the beginning of the session and at the first hour. Each HD session is assigned a new binary variable, IDH, that takes the value of "1" if there is a hypotension event and "0" if there is not. Finally, a new database, shown in Fig. 3, is formed containing the analytical and clinical variables associated with each session, keeping only the variables associated with the start of the HD session, the so-called "Hour 0".

This new database supports the goal of developing a predictive system that can accurately anticipate potential hypotensive episodes during dialysis sessions.

2.3 Data Processing and Variables Considered in the Clinical Study

After obtaining the integrated database, the medical staff, using their experience and clinical knowledge, determined a set of 67 variables to be considered for the predictive model to be developed. Subsequently, and as is usual in data science work, it is necessary to pre-process the data before starting the modeling phases. In the present case, after the tasks of integrating and combining data from different sources, cleaning tasks have been carried out, identifying and correcting possible errors in the data. For this purpose, an analysis of the variables to be analyzed was carried out, detecting possible quality problems in the data, and cleaning tasks were carried out in order to have a set of consistent data, correcting incorrect, atypical, or missing data. This data analysis process detected that many dialysis sessions or analytical tests lacked quality data. Therefore, the medical team opted to keep the largest number of variables to be considered for the models and to eliminate patients and dialysis sessions that lacked quality data so that finally, the data set used to run the predictive model considered 328 patients and a set of 68,574 sessions, which constitutes 69.96% and of which 19,810 sessions had IDH, representing 28.89% of the total number of HD sessions considered after the data cleaning process (Fig. 4). Both the patient cohort size and the number of HD sessions are representative of the population under study and allow for adequate modeling of the predictor system to be developed.

2.4 Enhanced Prediction of IDH Through Machine Learning and Biomarker Analysis

2.4.1 Machine Learning Model

To predict IDH, an XGBoost model was employed, selected for its superior performance in preliminary experiments compared to various methods, including KNN, Random Forest, and LGBM, as well as serving as a representative example of decision tree-based approaches. Initial hyper-parameter tuning was tailored to our dataset, which includes 67 features.

A 5-fold cross-validation technique was implemented to validate the model, ensuring robust performance evaluation.

Given the dataset's class imbalance, with only 28.89% of sessions representing the minority class (hypotensive patients), a data balancing technique called RandomUnderSampler was employed. This method was chosen based on previous experiments that demonstrated its superiority over RandomOverSampler and NearMiss techniques. The imbalance ratio was adjusted to 1:1, equalizing the number of samples in both the majority and minority classes, thereby improving the model's predictive accuracy.

2.4.2 Feature Selection with Metaheuristics

For feature selection, two representative metaheuristic algorithms were employed: Particle Swarm Optimization (PSO) and Grey Wolf Optimizer (GWO). PSO was selected as a classic metaheuristic model known for its effectiveness in solving optimization problems by simulating social behavior patterns. In contrast, GWO, inspired by the social hierarchy and hunting behavior of grey wolves, is recognized for its ability to balance exploration and exploitation during the optimization process. Both algorithms were chosen for their proven capability to efficiently navigate large search spaces and identify relevant features, thus enhancing the performance of the predictive model.

The binarization of solutions obtained from the metaheuristics was necessary to convert continuous variables into binary variables due to the discrete nature of the feature selection optimization problem. The S4 and STD transfer functions were employed

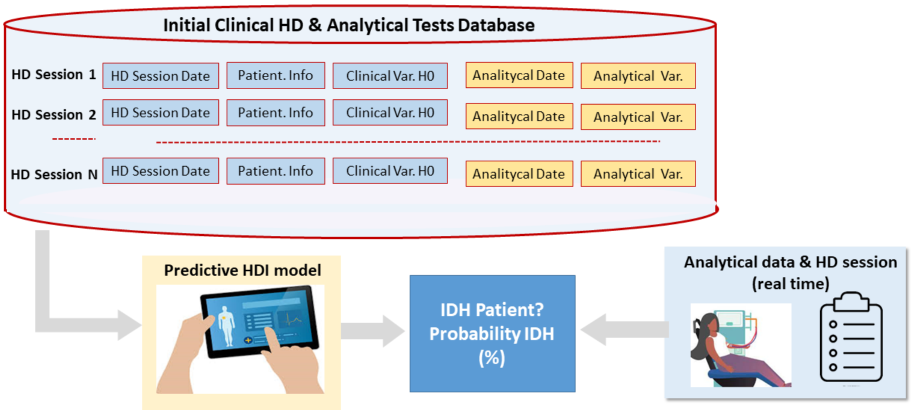

Figure 3: Predictive model at the start of the hemodialysis session.

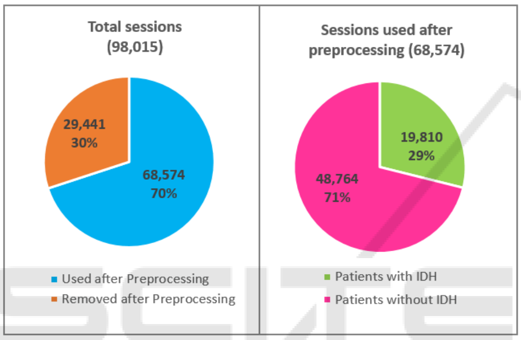

Figure 4: Number of HD sessions used to run the model.

for this process (Cisternas-Caneo et al., 2024).

The metaheuristic approach utilized two objective functions (Eq. 2), both incorporating the number of features in the model and various metrics to evaluate the classifier's performance, minimized over 100 iterations. The first version aimed to maximize the recall of the minority class (hypotensive patients) (Eq. 3), while the second focused on maximizing the F1-score of the minority class (Eq. 4). Additionally, the objective functions were weighted to favor performance metrics over feature reduction, allowing flexibility in adapting to the problem's nature.

$$\min z = 0.99 \cdot \text{Metric} + 0.01 \cdot \frac{\text{Selected features}}{\text{Total features}} \tag{2}$$

$$\text{Metric 1:} \quad 1 - \text{Minority Class Recall} \tag{3}$$

$$\text{Metric 2:} \quad 1 - \text{Minority Class F1-score} \tag{4}$$

where F1-score and recall are defined as:

$$\text{F1-Score} = \frac{TP}{TP + 0.5(FP + FN)}$$

$$\text{Recall} = \frac{TP}{TP + FN}$$

and TP is true positives, FN is false negatives and FP is false positives.

By iterating through these objectives, the metaheuristic algorithm effectively selected features that enhanced the model's predictive performance while addressing the dataset's class imbalance, as shown in Figure 5. Feedback from the classifier's performance metrics guided the metaheuristic process, representing a novel approach where the selection module integrates performance testing with various sets of variables chosen by the metaheuristic.

3 EXPERIMENTAL RESULTS

3.1 Initial Model Performance

Before applying metaheuristics algorithms for feature selection, the XGBoost model was trained using the complete set of 67 features. The initial performance metrics were as follows: an F1-score of 0.7172, precision of 0.7520, and recall of 0.7244. Given the nature of the problem, accurately predicting the minority class, i.e., hypotensive episodes, is critical. Therefore, the study primarily focused on metrics for the minority class. Specifically, the recall for the minority class was emphasized to minimize false negatives, which correspond to cases where hypotensive episodes are not predicted when they should be. Thus, the recall and F1-score for the minority class were the key metrics of interest, with values of 0.7541 and 0.6373, respectively.

3.2 Feature Reduction

Table 1 compares the performance of the XGBoost model using the original 67 features against the per-

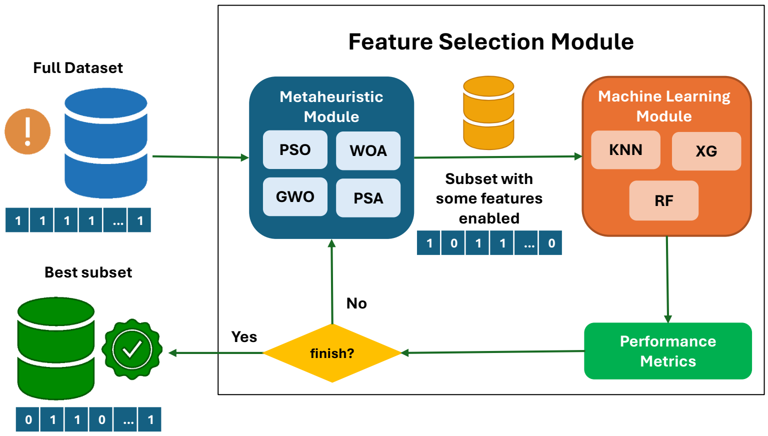

Figure 5: Feature selection process.

formance after feature reduction using PSO and GWO with both objective function metrics (Eq. 3, Eq. 4). The best results for the minority class F1-score and recall were achieved with the PSO algorithm using the first objective function (Eq. 3). Specifically, the minority class F1-score and recall values were 0.6419 and 0.7640, respectively. The feature selection process reduced the number of features to 36. Also using PSO algorithm for feature reduction achieved a 46.27% decrease in the initially selected features by the experts. Additionally, this process resulted in a slight improvement in the XGBoost model's performance for predicting hypotensive episodes in dialysis patients. Specifically, the F1-score for the minority class increased from 0.6373 to 0.6419, and the recall for the minority class improved from 0.7541 to 0.7640.

Fig. 6 presents the Receiver Operating Characteristic (ROC) curve for the IDH prediction model using the 36 features selected by PSO algorithm. The Area Under the Curve (AUC) value is 0.76.

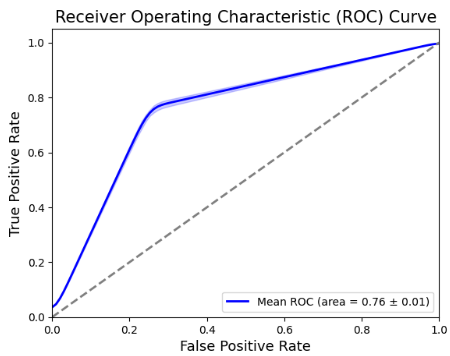

Figure 6: Receiver Operating Characteristic (ROC) curve and the area under the curve (AUC) for the XGBoost model trained with the 36 features chosen by the PSO model.

Fig. 7 shows the fitness evolution of the best solution over iterations for the PSO algorithm using the objective function that included the minority class recall as a metric (Eq. 3). The plot illustrates a gradual decrease in fitness, corresponding to an increase in the minority class recall. This trend indicates a reduction in false negatives and, consequently, an improvement in the predictive performance of the model.

4 CONCLUSION

Predicting hypotensive episodes in chronic kidney disease patients prior to dialysis is crucial for preventing complications and ensuring effective treatment. This study employed the XGBoost machine learning model to predict such episodes, initially using a dataset of 67 features selected by medical experts. Subsequently, metaheuristic algorithms, specifically PSO and GWO, were used to reduce the feature set and enhance the model's performance.

A key challenge in developing predictive models for medical applications is the large number of

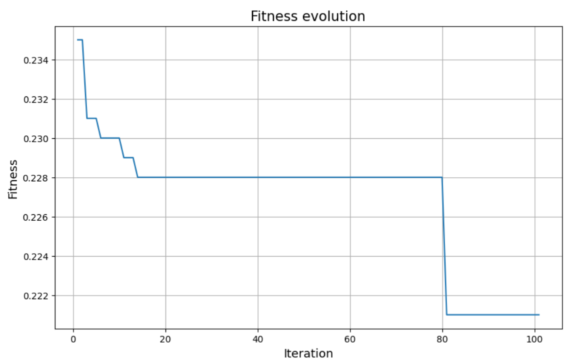

Figure 7: Fitness evolution.

Table 1: Classification results of models using Stratified k-fold cross-validation method.

Model	FO	IDH Patient			Non-IDH Patient			Accuracy	Total
	Metric	Recall	F1-score	Precision	Recall	F1-score	Precision		Features
NO	NO	0.7541 (0.007)	0.6373 (0.0060)	0.5518 (0.006)	0.7512 (0.004)	0.8116 (0.003)	0.8826 (0.003)	0.7520 (0.004)	67
PSO	1	0.7640 (0.015)	0.6419 (0.006)	0.5536 (0.005)	0.7497 (0.007)	0.8124 (0.003)	0.8867 (0.006)	0.7538 (0.004)	36
GWO	1	0.7617 (0.012)	0.6352 (0.006)	0.5448 (0.005)	0.7414 (0.006)	0.8067 (0.004)	0.8845 (0.005)	0.7473 (0.004)	38
PSO	2	0.7603 (0.008)	0.6422 (0.007)	0.5559 (0.007)	0.7532 (0.005)	0.8140 (0.004)	0.8855 (0.003)	0.7568 (0.006)	41
GWO	2	0.7560 (0.008)	0.6396 (0.009)	0.5527 (0.010)	0.7504 (0.009)	0.8119 (0.007)	0.8846 (0.004)	0.7547 (0.008)	38

NO, Without Metaheuristics; PSO, Particle Swarm Optimization; GWO, Grey Wolf Optimizer.

features, which can lead to increased computational complexity and potential overfitting. Effective feature reduction is essential to streamline the model, reduce computational load, and eliminate irrelevant or redundant information, thereby improving the model's performance and generalizability.

The study successfully developed a model capable of identifying IDH events in chronic kidney disease patients. By applying metaheuristic techniques, the number of features was significantly reduced, and the predictive accuracy of the model was improved. The PSO algorithm, in particular, demonstrated a robust reduction in the number of features, decreasing the feature set by 46.27% from the original 67 features to 36. This substantial reduction in features not only simplifies the model but also enhances its interpretability and efficiency. Reducing the number of features decreases the computational load, making the model faster and more efficient in processing data. Additionally, eliminating irrelevant and redundant information helps to avoid overfitting, thereby improving the model's generalizability. This streamlined approach also facilitates easier interpretation of the model's results, allowing for more straightforward insights into the key factors influencing IDH events.

This reduction in characteristics does not compromise the model's effectiveness. On the contrary, the optimized model achieved an AUC of 0.76, demonstrating its capability to distinguish between hypotensive and non-hypotensive episodes. Additionally, it achieved a recall of 0.764 for the minority class (hypotensive episodes) in chronic renal patients prior to dialysis procedures. This high recall value signifies a low number of false negatives, meaning that the model effectively identifies patients with IDH who might otherwise not be warned of such episodes. The improvement of recall and F1-score for the minority class, critical metrics for this medical prediction task, underlines the effectiveness of using metaheuristics and, in this case, PSO selects fewer significant features. Consequently, the optimized model not only provides reliable predictions of hypotensive episodes but also operates with greater efficiency, facilitating its potential integration into clinical practice.

In conclusion, this study highlights the importance of feature reduction in predictive modeling for medical applications. The use of metaheuristic algorithms, particularly PSO, has proven to be an effective strategy for enhancing model performance while significantly reducing the number of required features. This approach offers a promising pathway for developing efficient, accurate, and clinically applicable models for predicting hypotensive episodes in chronic kidney disease patients at the beginning of the HD session.

Looking ahead, there are several avenues for future research. Our model could be further refined by exploring additional machine learning techniques or ensemble methods combining different approaches. Extending the study to include predictions for other pathological events during dialysis, such as thrombosis and arrhythmias, could enhance its clinical utility. Additionally, incorporating the full initial dataset of 200 variables—beyond those selected by medical experts—and addressing missing data through imputation techniques would provide a more comprehensive analysis and potentially improve the model's predictive capabilities.

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