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Comparative evaluation of machine learning techniques for heart disease prediction using clinical data

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ABSTRACT

Heart disease remains one of the causes of death globally, making it very important to have an early diagnosis of the risks involved, thus helping with decisions and treatments of the patients. The current research work evaluates the performance of five algorithms for machine learning (ML): logistic regression (LR), Naïve Bayes (NB), random forest (RF), support vector machine (SVM), and extreme gradient boosting (XGBoost) in heart disease prediction using the Cleveland heart disease data from University of California, Irvine (UCI) ML repository. The data set contains 303 patient cases with 13 features. The performance indicators used include accuracy, precision, recall, F1-score, and receiver operating characteristic–area under the curve (ROC-AUC). NB algorithm produced the best accuracy and F1-score (81.97% and 84.51% respectively), while RF provided the best ROC-AUC (89.39%). The most significant attributes in terms of feature importance included chest pain type, ST segment (ST) depression, maximum heart rate, and number of major vessels. Therefore, it could be concluded that ML could aid in heart disease diagnosis and clinical decision support system. However, the use of a small data set from one source without validation limits the results' generalizability.

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1. INTRODUCTION

Currently, artificial intelligence (AI) and machine learning (ML) are becoming powerful tools for transforming the healthcare industry through predictive analysis, intelligent diagnostics, and clinical decision-support systems. The availability of large volumes of electronic health records (EHRs) and biomedical datasets has led to the development of data-based applications that can help predict certain diseases and support clinical decisions. Recently, some reviews have shown the increased application of ML for cardiovascular disease (CVD) prediction, which includes not only diagnosis but also clinical decision support and risk stratification [1]–[3]. CVD is one of the major challenges in global health, which causes significant mortality and is associated with modifiable risk factors such as smoking, physical inactivity, hypertension, diabetes, obesity, smoking, physical inactivity, and stress [4], [5].

ML is very appropriate for cardiovascular prediction since it can detect complicated relationships between clinical features. Recent studies have analyzed the efficiency of random forest (RF), logistic regression (LR), support vector machine (SVM), gradient boosting algorithms, Naïve Bayes (NB) and other classifiers for heart disease prediction [6]–[8]. Some comparative studies have also presented promising results from using different classification methods, although there is considerable variation depending on

dataset properties, preprocessing, feature selection, and evaluation methodology [7]–[10]. At the same time, the Cleveland Heart Disease dataset is one of the most commonly used datasets for evaluating classifiers' performances in this case [3], [11].

Current studies report high heterogeneity in predictors, preprocessing, validation, and evaluation of performance metrics, with insufficient external validation, which may pose questions on the generalizability [2], [9], [12], [13]. This fact adds to the need for a comparison study carried out under uniform experimental conditions. Interpretable ML models is an additional requirement for AI in healthcare. The clinician must be able to understand what predictors contributed to the prediction to incorporate ML models into the workflow of clinicians. Recent cardiovascular studies utilized explainable AI (XAI), feature importance techniques, SHapley Additive exPlanations (SHAP), and local interpretable model-agnostic explanations (LIME) in order to increase transparency and interpretability of models [10], [14], [15]. This way, clinically significant predictors can be selected and more information on model decisions will be obtained.

However, there is still a need for comparative studies under controlled conditions. Many recent papers utilize either small sample size, different preprocessing techniques, insufficient validation, or individual algorithms [2], [9], [12], [13]. It is challenging to define whether differences in results are caused by algorithms or experimental conditions.

Thus, this research provides a standardized comparative methodology for heart disease prediction through the Cleveland Heart Disease dataset available on the University of California, Irvine (UCI) ML repository. Five supervised ML algorithms; LR, SVM, RF, Naïve Bayes (NB) and extreme gradient boosting (XGBoost) are compared based on equal pre-processing and evaluation criteria. Predictive accuracy is measured in terms of accuracy, precision, recall, F1-score, and receiver operating characteristic–area under the curve (ROC-AUC), whereas permutation feature importance is calculated for determining key predictors.

2. MATERIALS AND METHOD

2.1. Research design

In this paper, a quantitative experimental design is used for the study on the effectiveness of ML algorithms through supervised learning for heart disease prediction. The study is conducted following a typical pipeline of ML process, which involves acquiring data, preprocessing data, exploratory data analysis (EDA), model development, evaluating models, and interpreting results [1], [2]. Data collection, preprocessing, EDA, scaling of features, splitting of the dataset, model training, evaluating models, feature importance analysis, and interpretation of models were part of the work flow. The study involves a binary classification task where the target variable is heart disease prediction.

2.2. Data source and dataset description

In the current research, the dataset to be used is the Cleveland Heart Disease dataset, which is found in the UCI ML repository [16]. The dataset contains 303 observations, 13 predictor variables, and one target variable. The predictor variables of the dataset are age, sex, chest pain type, resting blood pressure, serum cholesterol, fasting blood sugar, resting electrocardiographic results, maximum heart rate achieved, exercise-induced angina, ST depression (oldpeak), slope of ST segment, major vessels (ca), and thalassemia [16]. The dataset has been previously utilized for predicting heart disease in numerous previous studies [6], [7].

The target variable is coded from 0 to 4, where 0 indicates the absence of heart disease while 1 to 4 represents the presence of heart disease [16]. In the current research, the target variable is treated as a binary outcome variable.

$$Y = \begin{cases} 1, & \text{presence of heart disease} \\ 0, & \text{no heart disease} \end{cases} \quad (1)$$

2.3. Data preprocessing

In other to improve the data quality, data preprocessing was performed and prepare for the clinical variables modeling. Data preprocessing entailed missing value imputation, feature scaling, and distribution analysis of the classes [17].

2.3.1. Handling missing values

Missing values were noticed in the ca and thal features of the Cleveland dataset [16]. Median imputation was used for handling the missing values:

$$X_i = \begin{cases} \text{Median}(X), & \text{if } X_i \text{ is missing} \\ X_i, & \text{otherwise} \end{cases} \quad (2)$$

This method kept the existing observations without decreasing the sample size. Proper handling of missing values is significant for healthcare data sets since missing observations may influence future analysis and prediction [17].

2.3.2. Feature scaling

This normalization converts the variables into the interval [0, 1], which is especially important in the case of algorithms like LR and SVM that are impacted by the relative size of the features [18].

$$X_{scaled} = \frac{X - X_{min}}{X_{max} - X_{min}} \quad (3)$$

2.3.3. Class distribution analysis

Analysis of class distribution determined that there was no imbalanced distribution of positive and negative classes. Consequently, the use of methods such as synthetic minority over-sampling technique (SMOTE) was not needed.

2.4. EDA

EDA was performed to have an understanding of the statistics of the data set. The EDA process involved age distribution, gender distribution, descriptive statistics, correlation analysis, and relationships between features. Pearson's correlation coefficient was found to be:

$$r = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}} \quad (4)$$

This was done in order to gain an initial understanding of the relationship between these clinical variables.

2.5. Dataset splitting and validation strategy

A training dataset (80%) and a test dataset (20%) were separated for assessing the model's generalization capability:

$$D = D_{train} + D_{test} \quad (5)$$

For robustness, 5-fold cross-validation was performed while training the model. This makes for a more robust evaluation of the model's performance without the need to rely on one particular training set.

$$CV = \frac{1}{k} \sum_{i=1}^{k} Error_i \text{ , where } k = 5. \quad (6)$$

2.6. ML models

Five supervised ML models (SMLM) have been chosen for comparison because of their usage in healthcare predictive modeling and classification tasks [6]–[8].

2.6.1. LR

Heart disease probability is estimated using LR sigmoid function as:

$$P(Y = 1 \mid X) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 X_1 + \cdots + \beta_n X_n)}} \quad (7)$$

where β_0 represents the intercept and β_i represents the coefficient associated with predictor X_i.

2.6.2. NB

NB utilizes Bayes' theorem on the assumption of conditional independence of predictors:

$$P(C \mid X) = \frac{P(X \mid C)\, P(C)}{P(X)} \quad (8)$$

The procedure is computationally efficient and appropriate for the classification of relatively small datasets [6].

2.6.3. RF

RF consists of decision trees whose output class depends on majority voting as follows:

$$\hat{Y} = \text{Majority Vote } (T_1, T_2, \ldots, T_n) \quad (9)$$

The ensemble method improves generalization by aggregating predictions from several decision trees [7].

2.6.4. SVM

SVM constructs a decision boundary that separates classes:

$$w^T x + b = 0 \quad (10)$$

Non-linear relations between the input variables and the output were modeled using the radial basis function (RBF) Kernel.

2.6.5. XGBoost

XGBoost minimizes an objective function that consists of prediction loss and regularization:

$$Obj = \sum_{i=1}^{n} l(y_i, \hat{y}_i) + \sum_{k=1}^{K} \Omega(f_k) \quad (11)$$

The regularizer is responsible for managing the complexity of the model to prevent overfitting.

2.7. Hyperparameter configuration

To assure comparability, pre-defined hyperparameter settings for each particular model were used in all the experiments (Table 1).

Table 1. Hyperparameter configuration

Models	Parameters
LR	Solver = 'liblinear', max_iter = 1000
NB	GaussianNB default parameters
RF	n_estimators = 100, random_state = 42
SVM	Kernel = 'rbf', C = 1
XGBoost	Learning_rate = 0.1, max_depth = 3, n_estimators = 100

2.8. Model evaluation metrics

Model performance is measured by accuracy, recall, precision, F1 score, and ROC-AUC (Table 2). Accuracy is the measure of the overall accuracy of classification. Precision indicates the percentage of positives that have been classified accurately out of all predicted positives. Recall is the measure of the percentage of true positives that have been classified correctly. The ROC-AUC score is used to measure the classification discrimination capability of the model [9].

Table 2. Accuracy, precision, recall, and F1

Accuracy	Precision	Recall	F1-score
$\frac{TP + TN}{TP + TN + FP + FN}$	$\frac{TP}{TP + FP}$	$\frac{TP}{TP + FN}$	$2 \times \frac{Precision \times Recall}{Precision + Recall}$

TP: true positive, TN: true negatives, FP: false positives, and FN: false negatives

2.9. Feature importance analysis

Permutation feature importance method was applied to test the significance of each independent variable in the model.

$$Importance_j = Performance_{original} - Performance_{permuted} \quad (12)$$

A bigger drop in performance after permutation implies higher importance of the particular feature. This technique facilitates interpretation by pinpointing important clinical features.

2.10. Implementation Tools

The experiment was carried out in Python utilizing Jupyter Notebook. The experiment used libraries such as Scikit-learn [18], Pandas, NumPy, Matplotlib, Seaborn, and XGBoost. All experiments were carried out using the same computational setting and predetermined model settings.

3. RESULTS AND DISCUSSION

3.1. EDA results

EDA was performed to explore the statistical nature, distribution patterns, and correlation between the clinical variables before developing the model. EDA helps in detecting the patterns in the data, relationship between the features, and also the predictor of disease [19].

3.1.1. Age and gender distribution analysis and disease occurrence

Figure 1 displays the age distribution of the patients in the dataset. Most of the patients are within the 50-65 years age group, suggesting a predominance of middle-aged to elderly individuals in the dataset. This is in line with the fact that there is an increased risk of developing heart disease in old age [4]. Figure 2 displays the age distribution of heart disease according to gender. From the results, there is a higher occurrence of heart disease in men than women.

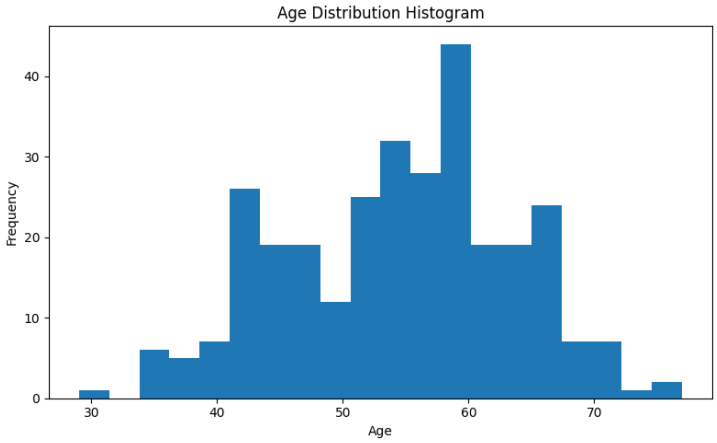


Figure 1. Age distribution histogram

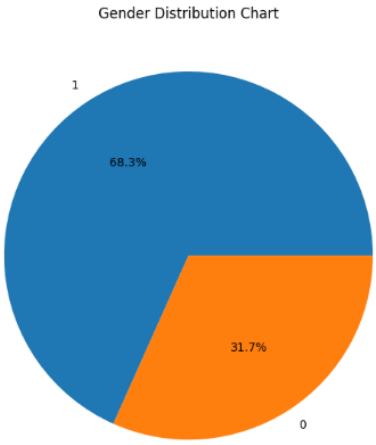


Figure 2. Gender distribution chart

3.1.2. Correlation analysis

The correlation heatmap between the clinical attributes and the target variable is shown in Figure 3. Type of chest pain (cp) and ST depression during exercise (oldpeak) appear to have a stronger correlation with heart disease, while maximum heart rate (thalach) is moderately correlated with heart disease. Such observations are significant from a clinical perspective since chest pain and exercise-induced ST-segment are significant signs when evaluating heart problems [20]. Characteristics like cholesterol and fasting blood glucose levels exhibit weak correlation with the target variable, which implies their inability to predict the dependent variable on their own.

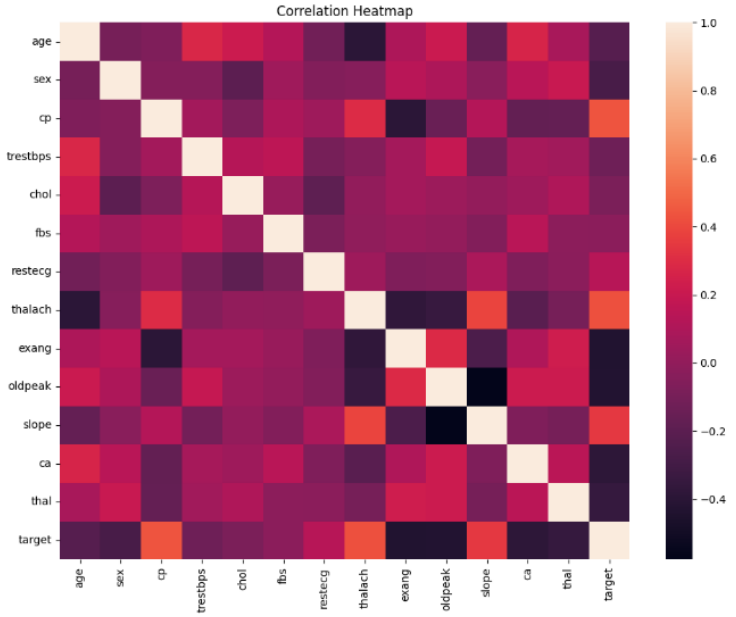


Figure 3. Correlation heatmap

3.1.3. Descriptive statistical analysis

Statistics for the distribution of certain clinical variables have been calculated. As can be seen from Table 3, there is great variability in the values of clinical measures, especially with regards to cholesterol levels, blood pressure, and maximum heart rate.

3.2. ML model performance evaluation

Five supervised ML models were compared based on accuracy, precision, recall, F1-score, and ROC-AUC. NB gave the highest accuracy (81.97%) and F1-score (84.51%), while RF gave the highest ROC-AUC (0.8939). This clearly shows that the best performing model is determined by the metric used to evaluate its performance. The figures in Table 4 are those used to evaluate the performance of the models on the held-out 20% test dataset. The five-fold cross validation technique was applied during the training process of the models.

Table 3. Descriptive statistics

Feature	Mean	Std. dev.	Min.	Max.
Age	54.37	9.08	29	77
Resting blood pressure	131.63	17.51	94	200
Cholesterol	247.03	52.56	126	564
Maximum heart rate	149.65	22.91	71	202
Oldpeak	1.04	1.16	0	6.2

Table 4. Comparative performance of ML models

Model	Accuracy	Precision	Recall	F1 score	ROC-AUC
LR	0.8033	0.8210	0.8350	0.8279	0.8550
NB	0.8197	0.8421	0.8480	0.8451	0.8626
RF	0.8033	0.8150	0.8310	0.8229	0.8939
SVM	0.7869	0.8030	0.8120	0.8075	0.8658
XGBoost	0.8033	0.8200	0.8270	0.8235	0.8582

NB showed the best performance concerning accuracy and F1-score, meaning that the algorithm demonstrated the best compromise between precision and recall. At the same time, the best ROC-AUC was shown by RF, which means that the algorithm has better discriminative ability in general. These discrepancies emphasize the need to use different metrics for model evaluation in healthcare [21].

3.2.1. ROC analysis

Figure 4 shows the ROC curves. RF achieved the highest ROC-AUC (0.8939), indicating the strongest discrimination across thresholds, although NB produced the highest accuracy and F1-score [21].

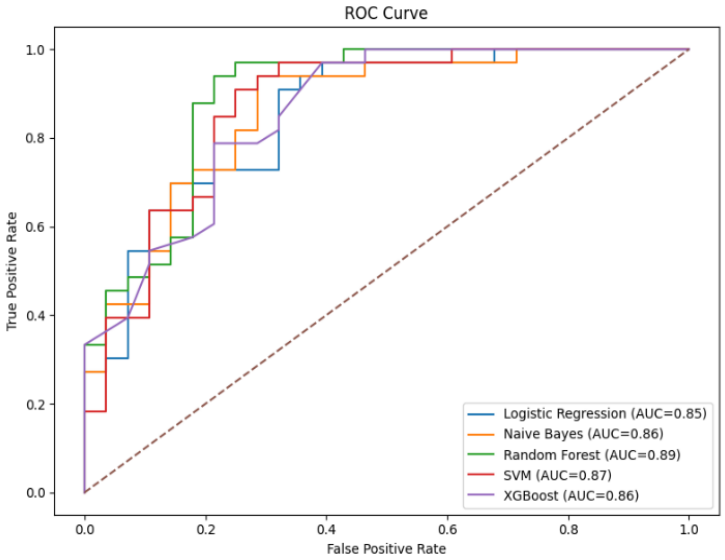


Figure 4. ROC curve

3.2.2. Confusion matrix analysis

Figure 5 presents the NB confusion matrix. Its high recall is relevant to screening applications, where missed positive cases may have serious consequences. The model nevertheless produced some false positives.

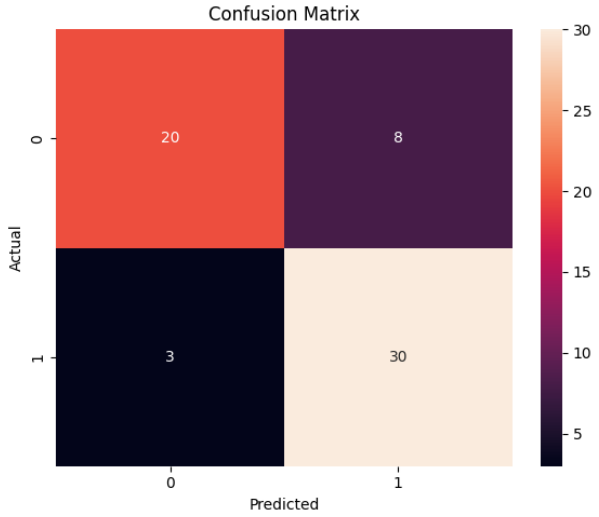


Figure 5. Confusion matrix

3.3. Feature importance analysis

Figure 6 shows the most influential features contributing to heart disease prediction. The most significant variables include chest pain type (cp), ST depression (oldpeak), maximum heart rate (thalach), and number of major vessels (ca). These features are consistent with established cardiovascular risk and diagnostic indicators [6], supporting the clinical interpretability of the model outputs.

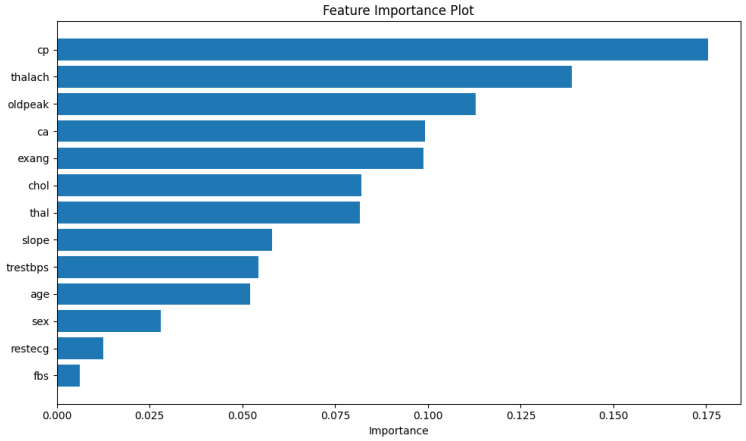


Figure 6. Feature importance plot

3.4. Discussion of findings

The outcome shows that all the five ML models can classify the heart disease well from the structured data. Among them, the NB model performed better compared to other ML models when accuracy and F1-score are the criteria. Similarly, the ROC-AUC of the RF was higher than others, suggesting that the superiority of the ML models is based on the criteria. In terms of the features, the significant ones are chest pain type, ST depression, maximum heart rate, and the number of major vessels, which are well-known indicators of the cardiovascular system [20]. Due to the small sample size and limited dataset from the Cleveland source, further studies have to include the other approaches like larger multicenter data and SHAP/LIME.

3.5. Recommendation

Further research must take into account the importance of having larger and diverse datasets that undergo external validation for increasing robustness and generalizability [22], [23]. The use of more clinical and longitudinal parameters could help in improving prediction, whereas the use of XAI tools such as SHAP and LIME could help in adding transparency [9], [24]. Future research could also examine ensemble learning techniques and deep learning along with calibration and clinical utility, consistent with recent evidence on the comparative use of ML techniques for heart disease prediction [25]. The integration with EHRs must be done only after adequate independent and prospective validation [20], [22].

4. CONCLUSION

The study examined the applicability of supervised ML methods in predicting heart disease with clinical data from the Cleveland Heart Disease dataset. Specifically, five algorithms (RF, LR, NB, SVM, and XGBoost) were tested under identical data pre-processing and evaluation processes. This type of comparison is important since contemporary studies stress the importance of the specific characteristics of the dataset, metric and validation methodology for the performance and clinical effectiveness of ML models.

The findings indicate that the best performance according to accuracy (81.97%) and F1-score (84.51%) was achieved by NB classifier, and the best ROC-AUC score was obtained by RF (0.8939). This indicates that model selection should not be based solely on one performance indicator, especially in medical applications since the discriminatory power, sensitivity, and predictive ability may mean different things. The outcomes of the study also confirm previous studies on the competitiveness of traditional ML methods for small-sized clinical datasets.

The feature importance study has shown that the chest pain type, ST depression, maximum heart rate, and the number of major vessels play an important role in the prediction process. Consistency with known cardiovascular criteria makes the interpretation of the results possible and strengthens the potential of ML in the context of clinical risk evaluation. Similar importance of interpretable ML approaches for cardiovascular prediction and clinical decision support was stated in recent studies.

It can be stated that the ML approach can be used in the detection of the heart disease risk and can serve as the basis for development of clinical decision support systems. Nevertheless, the small sample size of the Cleveland dataset reduces the generalizability of the results. Recently conducted research of AI in

cardiovascular domain has highlighted that high performance on internal data does not imply the high performance on the external data and external and multicenter validation is a crucial step in clinical application. Thus, the models suggested in this study should be considered as predictive research tools and not as clinically applicable diagnostic system.

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AUTHOR CONTRIBUTIONS STATEMENT

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C : **C**onceptualization
M : **M**ethodology
So : **So**ftware
Va : **Va**lidation
Fo : **Fo**rmal analysis
I : **I**nvestigation
R : **R**esources
D : **D**ata Curation
O : Writing - **O**riginal Draft
E : Writing - Review & **E**diting
Vi : **Vi**sualization
Su : **Su**pervision
P : **P**roject administration
Fu : **Fu**nding acquisition

CONFLICT OF INTEREST STATEMENT

Authors declare there is no conflict of interest. The authors confirm that they do not have any conflicts of interest that may seem to affect their research presented in this article.

DATA AVAILABILITY

The dataset used for this study is available openly on the UCI machine learning repository. The Cleveland Heart Disease dataset is found here: https://archive.ics.uci.edu/ml/datasets/heart+Disease. The processed dataset and results obtained from this study are available on request from the corresponding author.

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