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Corresponding Author	Family Name	**Shakhgeldyan**
	Particle	
	Given Name	**Karina I.**
	Prefix	
	Suffix	
	Role	
	Division	
	Organization	Far Eastern Federal University
	Address	Vladivostok, Russia
	Division	
	Organization	Vladivostok State University
	Address	Vladivostok, Russia
	Email	carinashakh@gmail.com
	ORCID	http://orcid.org/0000-0002-4539-685X
Author	Family Name	**Geltser**
	Particle	
	Given Name	**Boris I.**
	Prefix	
	Suffix	
	Role	
	Division	
	Organization	Far Eastern Federal University
	Address	Vladivostok, Russia
	Email	
	ORCID	http://orcid.org/0000-0002-9250-557X
Author	Family Name	**Rublev**
	Particle	
	Given Name	**Vladislav Yu.**
	Prefix	
	Suffix	
	Role	
	Division	
	Organization	Far Eastern Federal University
	Address	Vladivostok, Russia
	Email	

	ORCID	http://orcid.org/0000-0001-7620-4454
Author	Family Name	**Kuksin**
	Particle	
	Given Name	**Nikita S.**
	Prefix	
	Suffix	
	Role	
	Division	
	Organization	Far Eastern Federal University
	Address	Vladivostok, Russia
	Email	
	ORCID	http://orcid.org/0009-0005-9106-0117
Author	Family Name	**Pak**
	Particle	
	Given Name	**Regina L.**
	Prefix	
	Suffix	
	Role	
	Division	
	Organization	Far Eastern Federal University
	Address	Vladivostok, Russia
	Email	
	ORCID	http://orcid.org/0009-0004-3745-5399

Abstract	The aim of the study was to develop new prognostic models of postoperative atrial fibrillation (PoAF) in patients with ischemic heart disease (IHD) after coronary artery bypass grafting (CABG) based on preoperative predictors and to assess the effectiveness of their multilevel categorization to improve the quality of the prognosis and its clinical interpretation. A single-center retrospective cohort study was conducted, analyzing the data of 1305 medical histories of patients with IHD who underwent elective isolated CABG. Two groups were identified, the first group included 280 (21.5%) patients with PoAF, and the second group included 1025 (78.5%) patients without rhythm disturbances. Prognostic models of PoAF were developed using multifactorial logistic regression (MLR), random forest (RF), and stochastic gradient boosting (SGB) methods. The predictors were dichotomized using optimal cutoff points grid search methods, centroid calculation, and Shapley additive explanations (SHAP). For multilevel categorization, it was proposed to combine the threshold values identified during dichotomization and rank them based on cutoff thresholds using MLR weight coefficients (multi-metric categorization method). As a result of the multi-stage selection, 9 PoAF predictors were identified, validated and categorized. Prognostic models were developed with continuous, dichotomous, and multilevel categorical variables. The best SGB model with continuous predictors had an AUC of 0.795. Models with predictors identified by the multi-metric categorization method showed better performance than the models with continuous variables (AUC—0.802).

Keywords (separated by '-')	prognostic models - multilevel categorization - dichotomization - postoperative atrial fibrillation - stochastic gradient boosting - Shapley additive explanation (SHAP)

Predicting Atrial Fibrillation in Patients with Ischemic Heart Disease Based on Multilevel Categorization

Karina I. Shakhgeldyan[1,2](✉), Boris I. Geltser[1], Vladislav Yu. Rublev[1], Nikita S. Kuksin[1], and Regina L. Pak[1]

[1] Far Eastern Federal University, Vladivostok, Russia
carinashakh@gmail.com
[2] Vladivostok State University, Vladivostok, Russia

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A single-center retrospective cohort study was conducted, analyzing the data of 1305 medical histories of patients with IHD who underwent elective isolated CABG. Two groups were identified, the first group included 280 (21.5%) patients with PoAF, and the second group included 1025 (78.5%) patients without rhythm disturbances. Prognostic models of PoAF were developed using multifactorial logistic regression (MLR), random forest (RF), and stochastic gradient boosting (SGB) methods. The predictors were dichotomized using optimal cutoff points grid search methods, centroid calculation, and Shapley additive explanations (SHAP). For multilevel categorization, it was proposed to combine the threshold values identified during dichotomization and rank them based on cutoff thresholds using MLR weight coefficients (multi-metric categorization method).

As a result of the multi-stage selection, 9 PoAF predictors were identified, validated and categorized. Prognostic models were developed with continuous, dichotomous, and multilevel categorical variables. The best SGB model with continuous predictors had an AUC of 0.795. Models with predictors identified by the multi-metric categorization method showed better performance than the models with continuous variables (AUC—0.802).

Keywords: prognostic models · multilevel categorization · dichotomization · postoperative atrial fibrillation · stochastic gradient boosting · Shapley additive explanation (SHAP)

1 Introduction

Postoperative atrial fibrillation (PoAF) in patients with ischemic heart disease (IHD) is one of the most common complications of coronary artery bypass grafting (CABG) and occurs in 20–40% of patients [5, 15]. Despite numerous preventive strategies developed,

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the incidence of PoAF remains relatively constant [13, 18], but some authors noting a tendency for increased occurrence in the near future [3]. The negative consequences of PoAF are primarily associated with a 4-time increased risk of developing ischemic stroke and a 2-time increase in mortality at 30-day and 6-month observation periods [6]. The lack of a universal pathophysiological concept describing a single mechanism of PoAF development is the reason for creating forecasting tools to personalize the risk factors of this complication [7–9, 12].

Among the studies related to predicting PoAF, the POAF score scale developed using multifactorial logistic regression (MLR) and odds ratio calculation stands out. The insufficient performance of this scale prompted the expansion of predictor spectrum and the use of new machine learning (ML) methods, leading to an improvement in the quality metrics of PoAF prognostic models (AUC 0.7–0.75) [7, 19]. Predictors in these models were presented in both continuous and dichotomous forms, allowing the analyzed indicators to be classified as PoAF risk factors (e.g., age over 60 years). It is also worth noting that in previously published works, examples of clinical justification for the selection of threshold values allowing the personalization of PoAF risks and increasing the interpretability of model-generated conclusions were not presented when dichotomizing the data. In some studies, a multilevel categorization [19] was only used for the age indicator, with cutoff points arbitrarily set, for example, every 10 years after 60.

The aim of the study was to develop new prognostic models of PoAF in patients with IHD after isolated CABG based on preoperative predictors and evaluate the effectiveness of their multilevel categorization in enhancing the quality of prognosis and its clinical interpretation.

2 Methods

2.1 Study Population

The results of a single-center retrospective cohort study, which analyzed the medical history data of patients with ischemic heart disease (IHD) who underwent elective isolated coronary artery bypass grafting (CABG) at the cardio-surgical department of the State Budgetary Healthcare Institution "Primorsky Regional Clinical Hospital №1" in Vladivostok from 2008 to 2023, are presented. The dataset for analysis was formed from electronic medical records extracted from the hospital's medical information system. Patients with any form of atrial fibrillation (AF) in their medical history, as well as those who underwent CABG along with any other surgery, were excluded from the study. Thus, the dataset consisted of medical histories of 1305 patients (992 males and 313 females) aged 35 to 83 years. The study protocol complied with local institutional requirements and received full approval; patient consent was not required.

The primary endpoint was newly detected postoperative atrial fibrillation (PoAF). AF episodes lasting more than 30 s, verified by continuous electrocardiogram monitoring for at least 96 h after coronary artery bypass grafting (CABG), were considered as evidence of PoAF development. The cohort studied was divided into two groups. The first group included 280 (21.5%) patients who experienced AF episodes during the postoperative period in the hospital, and the second group included 1025 (78.5%) patients without arrhythmias. In the first group, hospital mortality was 7.8% (22 patients), while in the second group it was 3.7% (38 patients).

The preoperative clinical and functional status of the patients was assessed on the first day of hospital treatment using 130 factors, the main ones of which are presented in Table 1. Echocardiographic measurements were performed on a GE "Vivid-7" device according to the standard protocol [4]. The diameters of the left (LAD) and right atria (RAD), longitudinal dimensions of the left (LAL) and right atria (RAL), left ventricular internal diastolic (LVIDd) and systolic (LVIDs) dimension, as well as ECG results: durations of the RR, PQ, and QT intervals, P wave, and QRS complex, were analyzed.

2.2 Statistical Methods

The distribution of continuous variables according to the Kolmogorov-Smirnov test differed from normal, therefore non-parametric methods of mathematical statistics were used for them. The results were presented as median (Me) and interquartile ranges (Q1; Q3), and the Mann-Whitney test was used for intergroup comparisons of continuous variables, while the $\chi 2$ test was used for categorical variables. Odds ratios (OR) and their 95% confidence intervals (CI) were calculated for binary variables using Fisher's exact test. Differences were considered statistically significant at $p < 0.05$.

2.3 Supervised Machine Learning

Prognostic models for PoAF were developed using multiple linear regression (MLR), Random Forest (RF), and Extreme Gradient Boosting (XGBoost) decision tree models. The quality of these models was evaluated based on four metrics: area under the ROC curve (AUC), sensitivity (Sen), specificity (Spec), and F1-score. To select optimal hyperparameters, the Grid Search Cross-Validation (GridSearchCV) optimization method from the sklearn Python library was used.

The dataset was divided into two samples: one for training and cross-validation (80%) and the other for final testing (20%). The training and cross-validation procedure was performed using stratified k-Folders cross-validation on 10 folds. The average AUC quality metric was used for model selection, predictor selection and validation, and tuning of hyperparameters by exhaustive search over a grid of parameter values (GridSearchCV). For the final testing, the best MLR, RF, and GB models with optimal parameters and hyperparameters were trained on 80% of the dataset and evaluated on the final testing sample (20%).

To provide a reliable estimation of the quality metrics, the procedure was repeated 500 times with subsequent averaging of the metrics, initially splitting the data randomly using bootstrapping method.

2.4 Categorization of the Variables

In this research, a method of multilevel categorization was used, as previously reported by the authors [14].

To dichotomize potential predictors, we used optimization methods on the grid with a step of $\Delta = $ (max-min)/100: minimization of p-value - Min(p-value), maximization of

AUC—Max(AUC), quartile method, centroid method, and Shapley additive explanations (SHAP) [10]. The Shapley method allows identifying thresholds at which the predictor influence function on the endpoint demonstrated singularity, which may occur multiple times in the range of continuous feature values [14]. In order to perform multi-level categorization, we combined all threshold values identified through dichotomization using various methods, including the SHAP method. Close threshold values were merged through averaging. The centroid method assumed the use of the median of the analyzed features in comparison groups (with the PoAF feature and without the PoAF feature) and equally distant values (centroids), from which four categories were identified for each indicator [17]. The quartile method involves identifying four categories for each variable based on the evaluation of their medians, 2nd, and 3rd quartiles [12].

To assess the degree of influence of indicators on the endpoint, the Shapley method was applied.

2.5 Study Design

The research design consisted of 5 stages. In the first stage, after extracting data from the medical information system, a dataset was formed, which underwent procedures of verification, preprocessing, validation, and correction. Using intergroup comparison tests, a pool of potential predictors of PoAF was formed.

In the second stage of the study, prognostic models of PoAF with predictors in continuous form were developed using machine learning methods. The prognostic significance of the predictor was confirmed if its inclusion in the model led to an increase in the AUC value. All variables were considered in model development, regardless of statistical differences in comparison groups, and hyperparameter tuning was performed at this stage. Model development and cross-validation were carried out on 80% of the dataset (derivation cohort), and finally tested on 20% (validation cohort). The predictors and hyperparameters obtained at this stage were used for further steps.

In the third stage, binary categorization of continuous variables was carried out using different methods of threshold value determination, using the derivation cohort, and prognostic models of PoAF were developed based on this, validated on the validation cohort.

In the fourth stage of the study, multilevel categorization of variables was performed using four approaches. In the first approach, only thresholds identified by the SHAP method were considered, in the second approach—the set of threshold values obtained by other dichotomization methods was expanded. Additionally, thresholds obtained by the centroid method considering the medians of groups with and without PoFP, as well as using quartiles Q1, Q2, and Q3, were considered.

To assess the degree of risk factor influence on the endpoint, multiple linear regression models were developed, and their weight coefficients were used to encode multi-level categorical predictors. Risk factors with negative or close to 0 weight coefficient values in the multivariate linear regression model were excluded from consideration.

In the fifth stage of the study, four new prognostic models of PoAF were developed based on gradient boosting, with predictors obtained through different methods of multilevel categorization. Statistical significant differences in quality metrics were evaluated using bootstrapping method (n = 500), 95% CI, and comparison results using the Mann-Whitney test.

3 Results

3.1 Subject Characteristics

Analysis of clinical, demographic, and laboratory parameters between groups demonstrated that patients with PoAF were characterized by older age and an increased prevalence of tricuspid valve regurgitation (TR) among them (Table 1).

Table 1. Clinical and functional parametres of patients with IHD

Predictor	PoAF (n = 280)	Non-PoAF (n = 1025)	OR (95%) CI	p-value
Age, (y)	66 (61; 71)	63 (58; 69)	–	$<$ 0.000001
BMI, (kg/m^2)	27.97 (25.3; 31.2)	28.1 (25.1; 31.2)	–	0.736
LVIDs, (cm)	3.3 (3.2; 3.7)	3.35 (3; 3.8)	–	0.185
LVIDd, (cm)	5.1 (4.8; 5.425)	5.1 (4.7; 5.4)	–	0.284
LAL, (cm)	3.9 (3.6; 4.2)	3.9 (3.6; 4.3)	–	0.339
LAD, (cm)	4.6 (4; 5.1)	4.3 (3.8; 4.9)	–	0.0002
RAL, (cm)	3.8 (3.5; 4.1)	3.7 (3.4; 4)	–	0.0023
RAD, (cm)	4.5 (4.1; 4.9)	4.3 (3.8; 4.8)	–	0.0000033
P, (ms)	100 (100; 100)	100 (100; 100)	–	0.69
PQ, (ms)	160 (140; 180)	150 (140; 180)	–	0.025
QRS, (ms)	80 (80; 100)	80 (80; 100)	–	0.00036
RR, (ms)	950 (895; 1090)	900 (800; 1080)	–	0.129
QT, (ms)	400 (380; 430)	380 (360; 420)	–	0.00143
TR, n (%)	51 (18.21%)	112(10.93%)	1.8 [1.26; 2.6]	0.00154

Individuals in this group had higher values of LVIDs, LAD, RAD, and RAL, systolic pressure gradient LV/Ao, increased QT interval duration, and PQ.

3.2 Machine Learning Models

In the second stage of the research, prognostic models of PoAF were developed, validated, and tested using logistic regression, decision tree, and machine learning methods (Table 2).

For all models, the best results in terms of the AUC metric were obtained when ECG parameters (QRS, QT, PQ, RR intervals, and P wave), age, RAD, LVIDs, as well as hypertension were used as predictors.

Table 2. Performance assesment of prognostic models of PoAF using predictors in continuous form

Metrics	MLR	SGB	RF
AUC	0.698 [0.695; 0.702]	0.795 [0.791; 0.798]	0.779 [0.775; 0.782]
Sen	0.643 [0.636; 0.65]	0.718 [0.711; 0.725]	0.7[0.694; 0.707]
Spec	0.65 [0.647; 0.654]	0.72 [0.716; 0.723]	0.7 [0.697; 0.704]
F-score	0.416 [0.412; 0.42]	0.507 [0.503; 0.511]	0.485 [0.481; 0.488]

Comparing the predictive value of the developed models showed that SGB and RF methods provide higher prediction performance than MLR (AUC—0.698 vs 0.795 and 0.779).

3.3 Categorization

In the third stage of the research, the predictors of PoAF were dichotomized in continuous form using methods to search for an optimal cutoff threshold on a grid (Min(p-value) and Max(AUC)), by SHAP method, and by calculating the centroid (Table 3). The use of threshold values, deviation from which is associated with an increased probability of PoAF, allows considering binary data as risk factors for adverse events. The risk factor is encoded as "1" if the predictor value exceeds the threshold with a suffix "+", or does not reach it with a suffix "–", and "0" in all other cases.

Table 3. Dichotomization of continuous predictors of in-hospital mortality using various methods

Characteristics	Minimal p-value	Maximal AUC	Centroid	SHAP
Age, (y)	60.0+	60.0+	64.0+	61+
LVIDs, (cm)	3.0+	3.0+	3.35+	[3.1; 4.1] 5+
RAD, (cm)	4.12+	4.12+	4.4+	[4.2; 5.3]
QRS, (ms)	89-	89-	80-	80-
QT, (ms)	420+	382+	390+	390+
PQ, (ms)	163+	163.0+	155.0+	[170;210]
RR, (ms)	882.0+	882.0+	925.0+	[700; 750] [880; 1000] 1100
P, (ms)	120+	100++	100+	130+

The research results showed that the threshold values obtained through various binarization methods sometimes differed from each other. The first three dichotomization methods considered isolated indicators and did not take into account prognostic models. The SHAP method was applied to the multifactorial model of stochastic gradient boosting, and the threshold value was determined as the point where the SHAP value exceeded 0.2 units.

Prognostic models of PoAF with dichotomous predictors were developed based on MLR. It was found that the model obtained using the centroid method (AUC—0.689) significantly lagged behind models developed using Max(AUC) methods and SHAP, which have acceptable predictive ability (AUC: 0.736—0.791).

At the fourth stage of the research, four groups of PoAF risk factors were formed using various methods of multilevel categorization (Table 4).

Table 4. Weighting coefficients and thresholds of predictors obtained by multilevel categorization methods

Characteristics	SHAP		Multi-metric categorization		Group medians and centroid		Quartiles	
	Threshold	WC	Threshold	WC	Threshold	WC	Threshold	WC
Age, (y)	61+	0.63	60+	0.69	[63; 66] 66+	0.35 0.36	[58; 64] [64; 69] 69+	0.75 0.33 0.85
LVIDs, (cm)	[3.1; 4.1] 5+	1.03 1.23	[3.1; 4.1] 5+	1.0 1.15	[3.3; 3.35] 3.35+	0.83 0.17	[3.1; 3.3] [3.3; 3.8] 3.8+	1.93 1.18 1.42
RAD, (cm)	[4.2; 5.3]	0.46	[4.2; 5.3]	0.53	[4.3; 4.5] 4.5+	0.56 0.65	[3.8.4.3] [4.3; 4.8] 4.8+	0.91 1.38 0.88
QRS, (ms)	80–	0.92	80–	0.94	80–	0.98	[80; 100]	1.3
QT, (ms)	390+	1.03	390+	1.03	[380; 400] 400+	0.67 1.03	[360; 395] [395; 420] 420+	0.6 0.27 1.05
RR, мс	[700; 750] [880; 1000] 1100	1.31 1.21 2.33	[700; 750] [880; 1000] 1100	1.29 1.23 2.47	[900; 950] 950+	1.26 0.63	[800; 920] [920; 1080] 1080+	0.32 0.4 0.43
PQ, мс	[170; 210]	0.99	[170; 210]	1	160+	0.52	[140; 160] [160; 180] 180+	0.66 1.71 0.86
P, мс	130+	1.55	[100; 130] 130+	2.32 3.35	100+	5.89	100+	4.55
TR	1	0.68	1	0.7	1	0.79	1	0.72

The first pool of risk factors was obtained based on the analysis of SHAP values. The second pool expanded the first pool by adding threshold values obtained in the third stage of the study using several binarization methods. The third group of risk factors was represented by medians of predictors in comparison groups and their centroids, while the fourth group used threshold values corresponding to predictor quartiles.

To encode the values of multilevel categorical predictors, weighting coefficients (WC) from MLR models developed for each risk factor group were used. The approach that ensures the formation of the second pool of risk factors and their weighting coefficients is called multi-metric categorization.

3.4 Models Based on Multilevel Categorical Predictors

In the fifth stage, four prognostic models of PoAF were developed based on multilevel predictors obtained through various methods, using SGB (Table 5).

Table 5. Performance assessment of prognostic models of PoAF based on predictors with multilevel categorization

Metrics	Multilevel SHAP	Multi-metric categorization	Group medians and centroid	Quartiles
AUC	0.795 [0.77; 0.82]	0.802 [0.78; 0.82]	0.7 [0.67; 0.77]	0.66 [0.63; 0.69]
Sen	0.735 [0.67; 0.78]	0.741 [0.7; 0.78]	0.65 [0.61; 0.69]	0.6 [0.55; 0.65]
Spec	0.71 [0.688; 0.73]	0.713 [0.69; 0.73]	0.652 [0.63; 0.68]	0.618 [0.58; 0.66]
F-score	0.503 [0.47; 0.54]	0.507 [0.48; 0.53]	0.422 [0.4; 0.44]	0.31 [0.29; 0.34]

The model with predictors identified through multi-metric categorization demonstrated the best prognostic properties. It showed slightly better performance than the model that included continuous variables (AUC 0.8 vs. 0.791). The comparative performance assessment of prognostic models with predictors identified through dichotomization methods and multi-metric multilevel categorization showed the advantages of the latter, which was supported by statistically significant differences in the AUC metric (p-value < 0.001).

Using the SHAP and SGB methods, the degree of influence of individual predictors on PoAF development was evaluated. The QT interval showed the strongest influence (SHAP value—0.94) when exceeding the threshold of 450 ms, presence of TR, RR interval duration in the range of 700–1100 ms, and RAD of 4.2–5.3 cm. The low probability of PoAF development is associated with patients under the age of 60, LVIDs sizes up to 3 cm, and RAD up to 4.1 cm.

4 Discussion

Recently, prognostic models based on machine learning methods have been developed, the application of which in clinical practice is limited by the complexity of interpreting prognostic results. Promising tools to address this challenge are algorithms of explainable artificial intelligence (XAI), elements of which include determining threshold values of predictors and ranking them by the intensity of their impact on the endpoint. The determination of threshold values of predictors is performed through their categorization, which allows for detailing the relationships between clinical and functional status indicators of patients with the outcome variable. According to the literature, the most accessible method of multilevel categorization is descriptive statistics with the calculation of medians, quartiles, or quantiles [1, 11, 16]. However, a significant portion of critical remarks regarding categorization are associated precisely with this approach, primarily due to the dependency of these threshold values on the specific sample, lack of correlation with the clinical context, ignoring possible non-linear relationships, and others [11]. An alternative method that takes into account the clinical context is the search for optimal threshold values based on the minimization or maximization of target functions, for example, Min(p-value) or Max(AUC).

It has been determined that the SHAP method, which is considered as one of the promising XAI technologies, is a useful tool for categorization due to its efficient determination of cut-off thresholds, including for multilevel categorization and analysis of the relationship between predictors in continuous and categorical forms with the study endpoint. Potential risks of information loss when using new categorization methods have been overcome by detailing knowledge of the relationship between individual risk factors and the study endpoint. This was confirmed by comparing the quality criteria of prognostic models with predictors in continuous and multilevel categorical forms. Thus, for the best model with continuous predictors, the AUC was 0.795, and when using multi-metric categorization - 0.802.

It is also worth noting that our models had higher performance compared to those presented in a previously conducted study, in which only preoperative indicators and methods MLR, RF, and SGB were used (the best AUC in our study was 0.802 vs 0.74 in [7]). Significant differences are observed between the importance assessment using SHAP methods and weight coefficients for MLR. In our study, the highest importance for achieving the final endpoint based on the weight coefficients of MLR was associated with exceeding the value of P wave duration above 100 ms, while the highest risk according to the Shapley method was associated with QT $>$ 450 ms. The obtained results indicate the need for further research to assess the intensity of predictors' impact on the final endpoint, which is significant for the clinical interpretation of prognosis results.

5 Conclusion

In this study, based on a database of patients with IHD after isolated CABG machine learning methods (MLR, SGB, and RF) and 2 approaches to multilevel categorization of predictors of PoAF (multi-metric categorization and the SHAP method) were tested.

AQ4 Using the developed prognostic models for PoAF, it was shown that the categorization procedures proposed by the authors provide high performance and transparency of forecasting results.

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Declaration of Competing Interest. The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Chapter 21

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