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Deep learning for the prediction of acute kidney injury after coronary angiography and intervention in patients with chronic kidney disease: a model development and validation study

Ying Tang[a], Ting Wu[a], Xiufen Wang[a], Xi Wu[a], Anqun Chen[a], Guochun Chen[a], Chengyuan Tang[a], Liyu He[a], Yuting Liu[a], Meiyu Zeng[a], Xiaoqin Luo[b*] and Shaobin Duan[a*]

[a]Department of Nephrology, The Second Xiangya Hospital of Central South University; Hunan Key Laboratory of Kidney Disease and Blood Purification, Changsha, Hunan, China; [b]Department of Geriatrics, The Second Xiangya Hospital of Central South University, Changsha, Hunan, China

ABSTRACT

Background: Patients with chronic kidney disease (CKD) are considered the primary population at risk for post-contrast acute kidney injury (PC-AKI), yet there are few predictive tools specifically designed for this vulnerable population.

Methods: Adult CKD patients undergoing coronary angiography or percutaneous coronary intervention at the Second Xiangya Hospital (2015–2021) were enrolled. The patients were divided into a derivation cohort and a validation cohort based on their admission dates. The primary outcome was the development of PC-AKI. The random forest algorithm was used to identify the most influential predictors of PC-AKI. Six machine learning algorithms were used to construct predictive models for PC-AKI. Model 1 included only preoperative variables, whereas Model 2 included both preoperative and intraoperative variables. The Mehran score was included in the comparison as a classic postoperative predictive model for PC-AKI.

Results: Among the 989 CKD patients enrolled, 125 (12.6%) developed PC-AKI. In the validation cohort, deep neural network (DNN) outperformed other machine learning models with the area under the receiver operating characteristic curve (AUROC) of 0.733 (95% CI 0.654-0.812) for Model 1 and 0.770 (95% CI 0.695-0.845) for Model 2. Furthermore, Model 2 showed better performance compared to the Mehran score (AUROC 0.631, 95% CI 0.538-0.724). The SHapley Additive exPlanations method provided interpretability for the DNN models. A web-based tool was established to help clinicians stratify the risk of PC-AKI (https://xydsbakigroup.streamlit.app/).

Conclusion: The explainable DNN models serve as promising tools for predicting PC-AKI in CKD patients undergoing coronary angiography and intervention, which is crucial for risk stratification and clinical descion-making.

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Introduction

The advancements in coronary angiography and intervention have significantly improved both the diagnosis and prognosis of coronary heart disease [1,2]. Post-contrast acute kidney injury (PC-AKI) is characterized by a rapid decline in renal function that occurs after intravascular administration of iodinated contrast media [3]. It stands as one of the primary postoperative complications in patients undergoing coronary angiography (CAG) or percutaneous coronary intervention (PCI) [4,5]. Furthermore, PC-AKI is associated with prolonged hospitalization, increased medical costs, and increased risk of death, chronic kidney failure, and adverse cardiovascular events [6–8].

Renal insufficiency stands as a major risk factor for the development of PC-AKI [5,9]. Clinicians rely primarily on estimated glomerular filtration rate (eGFR) to identify individuals at high risk for PC-AKI [10–12]. Despite the diagnostic and therapeutic benefits of CAG/PCI [13,14], concerns regarding potential worsening renal function and the need for renal replacement therapy (RRT) following the procedure have resulted in its underutilization in patients with chronic kidney

CONTACT Shaobin Duan duansb528@csu.edu.cn Department of Nephrology, The Second Xiangya Hospital of Central South University; Hunan Key Laboratory of Kidney Disease and Blood Purification, Changsha, Hunan, China; Xiaoqin Luo luoxiaoqin@csu.edu.cn Department of Geriatrics, The Second Xiangya Hospital of Central South University, Changsha 410011, Hunan, China
*These authors contributed equally to this work and should be considered co-corresponding authors.
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disease (CKD) [15,16]. In this scenario, multivariable clinical predictive models are anticipated to serve as practical tools for stratifying the risk of PC-AKI. They can assist in clinical decision-making and preventive measures, such as administering low- or iso-osmolar contrast media, limiting the volume of iodinated contrast media, and ensuring adequate hydration [10,12]. Several predictive models have been established to predict the development of PC-AKI following coronary angiography and intervention procedures [17], yet few have specifically targeted patients with CKD. Additionally, most established models incorporated intraoperative variables such as contrast agent volume or the use of intra-aortic balloon pump (IABP), which are not applicable for preoperative risk assessment [17,18].

Machine learning (ML) is a branch of artificial intelligence that can automatically identify and analyze complex features from massive data. It excels at capturing non-linear trends and interactions within the data, thus improving predictive accuracy [19,20]. Deep learning is a subset of ML, fundamentally based on simulating the hierarchical structure of biological brains through multiple layers of artificial neural networks. This architecture enables each layer to learn increasingly abstract features from raw data, leading to significant breakthroughs in high-dimensional tasks such as image recognition, speech processing, and natural language understanding [21]. The deep neural network (DNN) is currently one of the most popular and effective neural network architectures, characterized by its multiple hidden layers [22]. Our previous study revealed that DNN models significantly outperformed logistic regression models in predicting acute kidney injury (AKI) following the intravenous administration of iodinated contrast media [23]. Additionally, Le et al. developed a predictive model for AKI in critically ill patients based on the convolutional neural network algorithm, which exhibited superior predictive performance compared to the extreme gradient boosting (XGBoost) algorithm [24].

Therefore, the study aimed to develop and validate ML models to predict PC-AKI in CKD patients undergoing coronary angiography and intervention procedures. Six ML algorithms, including DNN, naive Bayes (NB), k-nearest neighbors (KNN), logistic regression (LR), random forest (RF) and XGBoost, were employed and compared to identify the most effective predictive model. Our goal was to establish two models: one based exclusively on preoperative variables and the other combining preoperative and intraoperative variables, to assist in risk stratification and clinical decision-making both before and after the procedure.

Methods

Study design and population

The retrospective study identified adult patients (aged ≥ 18 years) with CKD (defined as eGFR < 60 mL/min/1.73 m^2) who underwent CAG or PCI at the Second Xiangya Hospital of Central South University between January 1, 2015 and December 31, 2021. The eGFR was calculated using the Chronic Kidney Disease Epidemiology Collaboration (CKD-EPI) equation [25]. The exclusion criteria were: (1) patients with end-stage renal disease (eGFR < 15 mL/min/1.73 m^2), chronic dialysis, or renal transplantation; (2) patients with missing serum creatinine (SCr) measurement either before or within 72 h after the procedure; (3) patients exposed to iodinated contrast media or surgical procedures within 72 h before or after CAG/PCI. The dataset was divided into a derivation cohort and a validation cohort based on patients' admission dates. The derivation cohort included patients admitted between January 1, 2015 and December 31, 2020, while the validation cohort comprised patients admitted between January 1, 2021 and December 31, 2021. This study was approved by the medical ethics committee of the Second Xiangya Hospital of Central South University (No.2022-K031). Written informed consent was waived for this retrospective analysis. The study was performed in accordance with the Declaration of Helsinki.

Outcomes

The primary outcome was the occurrence of PC-AKI, which was defined according to the European Society of Urogenital Radiology (ESUR) guidelines as an increase in SCr ≥ 26.5 μmol/L or ≥ 1.5 times the baseline value within 72 h after the administration of contrast media [3]. The baseline SCr level was defined as the preoperative measurement closet to the procedure. PC-AKI stage 1 was defined as an increase in sCr by ≥ 0.3 mg/dL (≥ 26.5 μmol/L) or to 1.5-1.9 times baseline, stage 2 as an increase in sCr to 2.0-2.9 times baseline, and stage 3 as an increase in sCr to ≥ 4.0 mg/dL (≥ 354 μmol/L) or to ≥ 3.0 times baseline, or the initiation of RRT. Secondary outcomes included Major Adverse Kidney Events within 30 days (MAKE30) and all-cause mortality within 30 days, 90 days, and 1 year. MAKE30 was defined as the occurrence of any of the following before discharge or within 30 days after CAG/PCI (whichever occurs first): death, initiation of RRT, and persistent renal dysfunction [26]. Initiation of RRT was defined as patients who did not receive RRT before CAG/PCI but initiated RRT after the procedure. Persistent renal dysfunction was defined as the last inpatient SCr measurement being ≥ 200% of the baseline SCr. Mortality data were collected from the Chinese Center for Disease Control and Prevention cause-of-death reporting system, a national administrative registry responsible for the collection and management of death information from all provinces in China.

Predictor variables

Predictor variables considered to be associated with PC-AKI were categorized into preoperative and intraoperative stages and extracted from electronic medical records. Preoperative features ($n = 34$) included demographics, comorbidities, laboratory variables, and medications. The preoperative variables were collected during the period from admission to the procedure. Intraoperative features ($n = 5$) contained the use of IABP, PCI, vasoactive drugs, contrast volumes, and emergency

procedure. Comorbidities were identified based on discharge diagnoses, which were coded using the International Classification of Diseases (ICD)-10 classification system. We categorized the comorbidities according to the Charlson Comorbidity Index (CCI), a widely used tool in recent studies for assessing the burden of comorbid conditions [27,28]. The preoperative measurements closest to the time of CAG/PCI were used for laboratory variables. All patients with renal insufficiency received guideline-recommended treatment, including routine intravenous hydration [12]. Moreover, physicians would adjust treatment based on the specific clinical condition of each patient. Medications were recorded based on the medication exposure within 3 days preceding the procedure.

Data processing and feature selection

Variables with more than 20% missing data were excluded. For the remaining variables, missing values were imputed using the random forest imputation method with the R package missForest (version 1.5) [29]. Missing values in this study are shown in Supplementary Table S1. Given the severe class imbalance in the derivation cohort, which could impact the models' learning ability, we applied the Synthetic Minority Over-sampling Technique (SMOTE) to adjust the ratio of PC-AKI patients to no PC-AKI patients to 1:1. This adjustment was performed using the Python package imbalanced-learn, version 0.8.1. Additionally, continuous variables were normalized before training to mitigate the impact of varying scales and ranges. Near-zero variance variables were eliminated to maximize the effectiveness of the features and simplify the model. The RF algorithm was utilized to assess the importance of each feature for PC-AKI prediction, ranking candidate variables based on their importance to identify the most predictive ones.

Model training and selecting

Two separate models were developed. Model 1 incorporated only preoperative features selected by the RF model, whereas Model 2 additionally included intraoperative features, all of which were identified as independent predictors of PC-AKI in previous studies [18,30,31]. Six ML algorithms were used to establish the predictive model, including DNN, NB, KNN, LR, RF, and XGBoost. The Mehran risk score was included in the comparison as a classic postoperative predictive model for PC-AKI. It incorporates eight clinical variables: hypotension, IABP, congestive heart failure, SCr or eGFR level, diabetes, age over 75 years, anemia, and contrast media volume [18].

DNN is a multi-layer neural network consisting of an input layer that receives data, several hidden layers that extract features through weighted connections and non-linear activation functions, and an output layer that generates the final predictions based on the learned representations [22]. Here, using TensorFlow (version 1.14.0) as the backend and Keras API (version 2.3.1) as the frontend, a DNN architecture was constructed. Four fully connected hidden layers were contained in the model, each employing the Rectified Linear Unit (ReLU) activation function for non-linear transformation, with the dropout layer followed to prevent overfitting. The output layer utilized the sigmoid activation function to generate the predicted probability of PC-AKI. The model compiled using the Adam optimizer with binary cross-entropy as the loss function. NB is a straightforward probabilistic classifier based on Bayes' theorem and the assumption of conditional independence among features [32]. The algorithm calculates the probability of each class based on the input features and selects the class with the highest probability as its prediction. However, its performance may be limited by its strong assumption of feature independence. LR is a statistical classification algorithm that constructs a linear regression model to quantify the relationship between input features and the outcome [33]. It then applies the sigmoid function to transform this linear combination into a probability, thereby predicting the likelihood of a binary outcome. KNN is a non-parametric method applicable to both classification and regression tasks. It calculates the spatial distance between the test sample and all training samples, identifying the K closest samples as its nearest neighbors [34]. The algorithm then utilizes their labels or values to make predictions for classification or regression. RF is a tree-based ML algorithm that integrates predictions from multiple decision trees through majority voting to enhance the accuracy of prediction [35]. XGBoost is an advanced gradient boosting algorithm that utilizes an ensemble of decision trees to enhance predictive accuracy [36]. It iteratively constructs each tree to predict the residuals from previous trees, with the goal of minimizing a loss function that measures prediction error. XGBoost improves performance by employing L1 and L2 regularization to mitigate overfitting, while also supporting parallel processing to handle large datasets efficiently. The NB, LR, KNN, RF, and XGBoost models were constructed using the scikit-learn package in Python 3.6. All models mentioned utilized 5-fold cross-validation for hyper-parameter tuning.

Model evaluation and web app development

Model discrimination was evaluated by the area under the receiver operating characteristic curve (AUROC), which served as the primary metric for evaluating model performance. The area under the precision-recall curve (AUPRC) was also calculated, as it is considered a valuable performance metric for imbalanced data. For the final models, we selected the cutoff value that maximized sensitivity while maintaining specificity above 60% as the optimal cutoff, aiming for more sensitive identification of PC-AKI patients. We then calculated the sensitivity, specificity, positive predictive value, negative predictive value, positive likelihood ratio, and negative likelihood ratio at this cutoff. Decision curves were used to assess the clinical utility of the predictive models, providing a quantitative evaluation of its potential impact on patient care decisions. We further conducted a sensitivity analysis to evaluate the robustness of the prediction models. Patients were stratified based on eGFR levels, age, gender, and comorbidities,

and the models' performance was assessed across these subgroups. Furthermore, we used the SHapley Additive exPlanations (SHAP) method to explore the interpretability of the DNN models. SHAP is a game theoretic approach that helps in explaining the output of any ML model. It provides a way to understand the contribution of each feature to the model's output, offering insights into the decision-making process of the DNN models [37]. Finally, we developed a user-friendly online tool based on the best-performing models to predict the risk of PC-AKI automatically, aiming to facilitate its widespread clinical application.

Statistical analysis

The Shapiro–Wilk test was used to assess the normality of continuous variables. Variables with a normal distribution were expressed as mean ± SD and compared using the Student's *t*-test. Variables with a non-normal distribution were presented as median with interquartile range (IQR), and comparisons were made using the Mann–Whitney U-test. Categorical variables were expressed as n (%) and were compared by the χ^2 test or Fisher's exact test as appropriate. Kaplan–Meier analysis was used to calculate cumulative mortality over time, and comparisons were performed using the log-rank test. R 4.2.3 and Python 3.6 were used for statistical analysis. A two-sided *p*-value of less than 0.05 was considered statistically significant.

Result

Baseline characteristics

A total of 989 patients with CKD were included in the study, with 725 in the derivation cohort and 264 in the validation cohort. Details for patient selection are provided in Figure 1. Baseline characteristics of each cohort are listed in

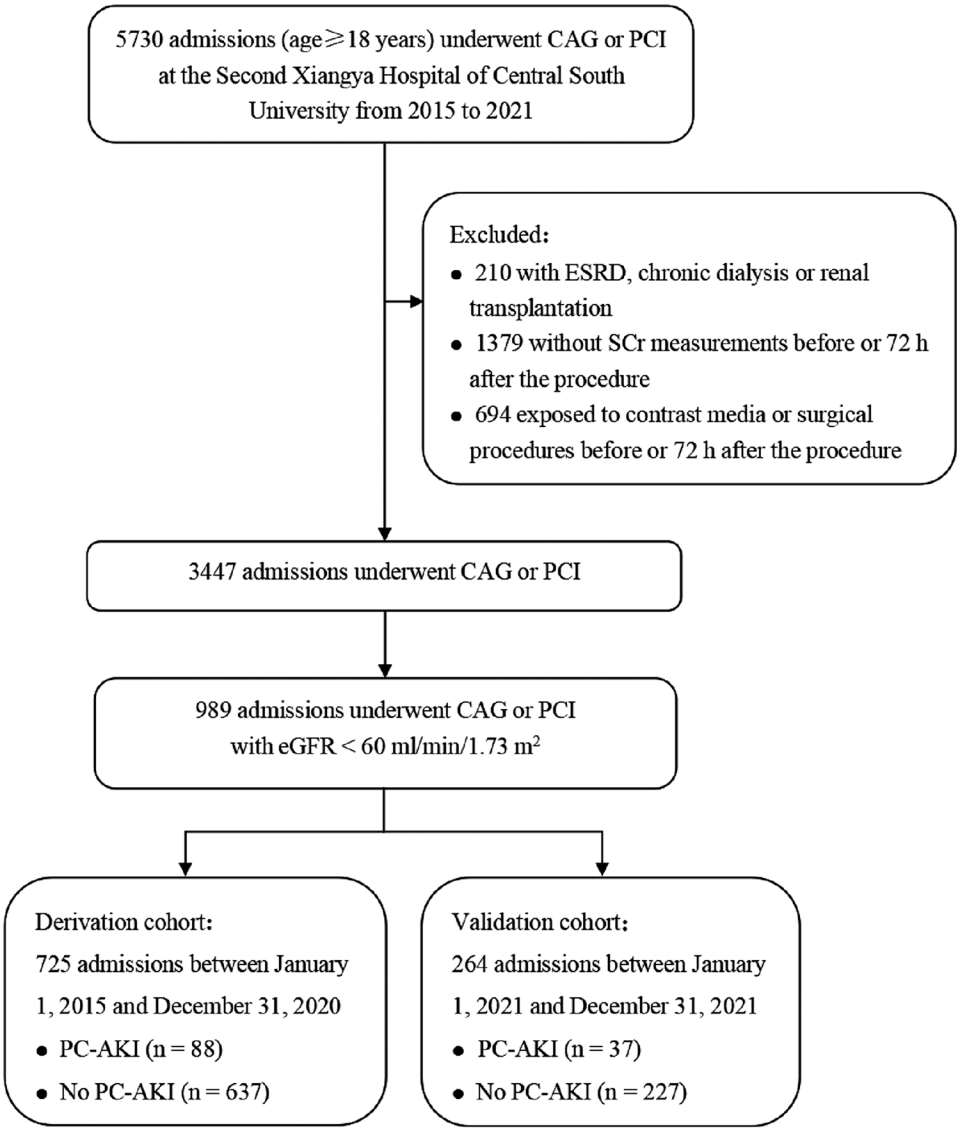

Figure 1. Flowchart of patient selection. Abbreviations: CAG, coronary angiography; PCI, percutaneous coronary intervention; ESRD, end-stage renal disease; SCr, serum creatinine; eGFR, estimated glomerular filtration rate; PC-AKI, post-contrast acute kidney injury.

Supplementary Table S2. Overall, the median age was 69 (IQR, 63-75) years, and 712 (72.0%) were male. The median baseline SCr was 135.0 (IQR, 114.9-163.7) μmol/L and the median baseline eGFR was 44.5 (IQR, 34.5-52.4) ml/min/1.73 m^2. There were 125 (12.6%) patients who developed PC-AKI, among whom 107 (85.6%), 7 (5.6%), and 11 (8.8%) patients developed PC-AKI stages 1, 2, and 3, respectively. Baseline characteristics of patients with and without PC-AKI are listed in Table 1. Compared to patients without PC-AKI, those who developed PC-AKI exhibited a higher prevalence of diabetes and myocardial infarction. Patients with PC-AKI had lower levels of hemoglobin, as well as higher levels of red cell distribution width-coefficient of variation (RDW-CV), urine protein, N-terminal pro-B-type natriuretic peptide (NT-proBNP), creatine

Table 1. Baseline characteristics of patients with and without PC-AKI.

Variables	No PC-AKI (*n* = 864)	PC-AKI (*n* = 125)	*P* value
Age, years	69 (63–75)	68 (63–74)	0.621
Male sex, n (%)	622 (72.0)	90 (72.0)	1.000
Comorbidities, n (%)			
Diabetes	356 (41.2)	74 (59.2)	<0.001
Hypertension	656 (75.9)	101 (80.8)	0.276
Arrhythmia	300 (34.7)	50 (40.0)	0.292
Myocardial infarction	443 (51.3)	90 (72.0)	<0.001
Congestive heart failure	531 (61.5)	86 (68.8)	0.138
Peripheral vascular disease	204 (23.6)	31 (24.8)	0.858
Cerebrovascular disease	142 (16.4)	28 (22.4)	0.127
Chronic lung disease	135 (15.6)	21 (16.8)	0.837
Liver disease	107 (12.4)	16 (12.8)	1.000
CCI score	3 (2–5)	5 (3–6)	<0.001
Laboratory data at baseline			
SCr, μmol/l	135.0 (114.9–163.0)	135.4 (115.4–172.1)	0.333
eGFR, ml/min/1.73 m^2	44.6 (34.8–52.7)	43.8 (33.3–50.1)	0.232
blood urea nitrogen, mmol/l	8.8 (6.8–11.3)	9.3 (7.5–11.4)	0.178
Uric acid, μmol/l	438.0 (362.2–522.0)	429.3 (365.4–530.5)	0.925
Hemoglobin, g/l	119 (106–133)	111 (99–127)	<0.001
White blood cell,10^9/l	6.7 (5.5–8.3)	7.1 (5.5–8.6)	0.283
Platelet count,10^9/l	200 (161–250)	193 (161–252)	0.751
RDW-CV, %	13.3 (12.7–14.1)	13.7 (12.9–14.7)	0.004
Urine protein, n (%)			0.001
–/+–	580 (76.2)	65 (60.7)	
+	88 (11.6)	14 (13.1)	
2+	66 (8.7)	22 (20.6)	
3+	24 (3.2)	4 (3.7)	
4+	3 (0.4)	2 (1.9)	
Serum albumin, g/l	35.4 (32.5–38.3)	34.9 (32.0–37.3)	0.087
TBIL, μmol/l	9.5 (7.0–13.2)	8.5 (6.5–11.6)	0.025
ALT, U/l	19.4 (13.5–30.4)	17.7 (11.7–31.4)	0.146
AST, U/l	21.3 (16.7–31.2)	21.4 (15.8–35.6)	0.919
Serum potassium, mmol/l	4.2 (4.0–4.6)	4.3 (4.0–4.6)	0.593
Serum sodium, mmol/l	140.0 (138.0–142.2)	140.3 (138.1–142.0)	0.835
Serum chlorine, mmol/l	104.2 (101.4–106.7)	104.4 (101.6–107.0)	0.495
Serum calcium, mmol/l	2.2 (2.1–2.2)	2.1 (2.1–2.2)	0.283
APTT, s	37.2 (33.0–41.6)	38.4 (33.5–42.7)	0.075
Creatine Kinase, U/l	73.2 (49.0–114.3)	81.0 (56.9–144.6)	0.022
Creatine kinase-MB, U/l	13.7 (10.6–17.9)	14.8 (11.2–20.9)	0.043
Cardiac troponin T, pg/ml	31.4 (17.0–113.6)	89.7 (33.8–437.2)	<0.001
NT-proBNP, pg/ml	1,877.0 (561.0–4733.0)	3,934.8 (1355.4–8328.5)	<0.001
LVEF, %	53 (40–60)	52 (40–57)	0.150
Medications before procedures, n (%)			
Digoxin	91 (10.5)	16 (12.8)	0.543
Diuretics	481 (55.7)	91 (72.8)	<0.001
ACEI/ARB	491 (56.8)	66 (52.8)	0.452
NSAIDs	597 (69.1)	91 (72.8)	0.461
Nephrotoxic antibiotics	4 (0.5)	0 (0.0)	0.993
β-blockers	611 (70.7)	92 (73.6)	0.576
Statins	752 (87.0)	107 (85.6)	0.762
Procedural features			
Emergency procedure, n (%)	29 (3.3)	20 (16.0)	<0.001
PCI, n (%)	451 (52.2)	81 (64.8)	0.011
IABP, n (%)	42 (4.9)	16 (12.8)	0.001
Contrast volume, ml	100 (50–200)	100 (100–200)	0.028
Vasoactive drugs, n (%)	35 (4.1)	14 (11.2)	0.001
Mehran score	11 (8–15)	13 (10–17)	<0.001

Abbreviations: CCI, Charlson Comorbidity Index; SCr, serum creatinine; eGFR, estimated glomerular filtration rate; RDW-CV, red cell distribution width-coefficient of variation; TBIL, total bilirubin; ALT, alanine aminotransferase; AST, aspartate aminotransferase; APTT, activated partial thromboplastin time; NT-proBNP, N-terminal pro-B-type natriuretic peptide; LVEF, left ventricular ejection fraction; ACEI, angiotensin-converting enzyme inhibitor; ARB, angiotensin receptor blocker; NSAIDs, non-steroidal anti-inflammatory drugs; PCI, percutaneous coronary intervention; IABP, intra-aortic balloon pump.

kinase, creatine kinase-MB, and cardiac troponin T compared to those without PC-AKI. Patients with PC-AKI were more likely to undergo emergency procedures, PCI, IABP, and received a higher volume of contrast media during the procedures. Additionally, they presented with higher CCI and Mehran scores and a greater proportion of diuretic use prior to the procedures.

Outcomes

The outcomes of patients with and without PC-AKI are listed in Table 2. Compared to patients without PC-AKI, those who suffered PC-AKI had a significantly higher incidence of MAKE30 (1.6% vs. 16.8%, $p<0.001$) and increased all-cause mortality at 30 days (1.3% vs. 5.4%, $p=0.009$), 90 days (2.9% vs. 11.7%, $p<0.001$), and 1 year (6.7% vs. 22.5%, $p<0.001$). Kaplan-Meier curves illustrating the unadjusted relationships between observed PC-AKI and subsequent death within 30 days, 90 days, and 1 year are presented in Figure 2.

Table 2. Outcomes of patients with and without PC-AKI.

Variables	No PC-AKI ($n=864$)	PC-AKI ($n=125$)	*P* value
MAKE30, n (%)			
Death	3 (0.3)	1 (0.8)	1.000
Initiation of RRT	11 (1.3)	12 (9.6)	<0.001
Persistent renal dysfunction	2 (0.2)	9 (7.2)	<0.001
Composite outcome	14 (1.6)	21 (16.8)	<0.001
Death at 30 days, n (%)	10 (1.3)	6 (5.4)	0.009
Death at 90 days, n (%)	22 (2.9)	13 (11.7)	<0.001
Death at 1 year, n (%)	51 (6.7)	25 (22.5)	<0.001

Abbreviations: MAKE30, major adverse kidney events within 30 days; RRT, renal replacement therapy.

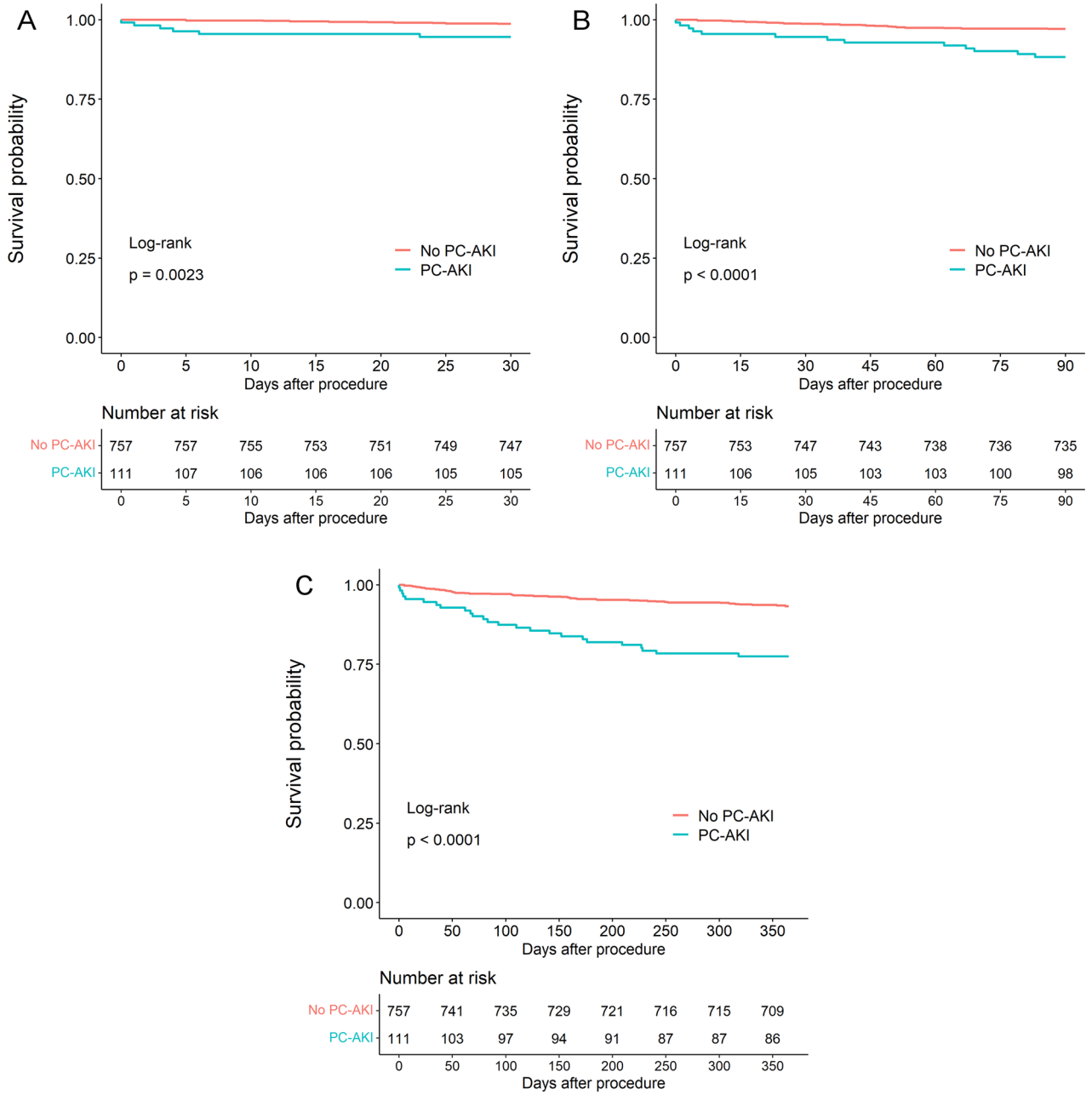

Figure 2. Kaplan–Meier Survival curves of patients with and without PC-AKI. Abbreviations: PC-AKI, post-contrast acute kidney injury.

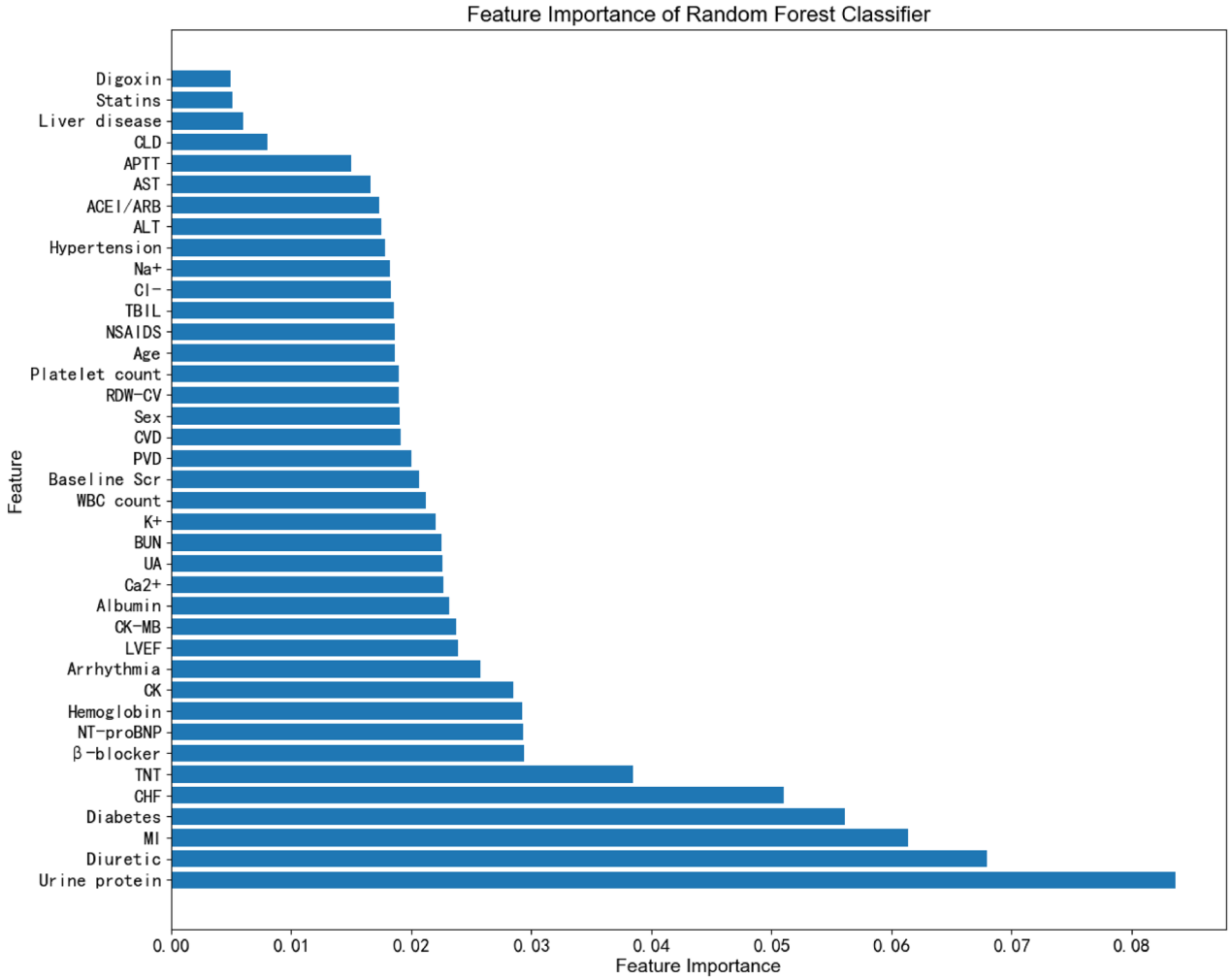

Figure 3. Feature importance for PC-AKI prediction generated by the RF model. Abbreviations: MI, myocardial infarction; CHF, congestive heart failure; TNT, cardiac troponin T; NT-proBNP, N-terminal pro-B-type natriuretic peptide; CK, creatine kinase; LVEF, left ventricular ejection fraction; CK-MB, creatine kinase-MB; UA, uric acid; BUN, blood urea nitrogen; WBC, white blood cell; SCr, serum creatinine; PVD, peripheral vascular disease; CVD, cerebrovascular disease; RDW-CV, red cell distribution width - coefficient of variation; NSAIDs, non-steroidal anti-inflammatory drugs; TBIL, total bilirubin; ALT, alanine aminotransferase; ACEI/ARB, angiotensin-converting enzyme inhibitor/angiotensin receptor blocker; AST, aspartate aminotransferase; APTT, activated partial thromboplastin time; CLD, chronic lung disease.

Feature selection

Figure 3 shows the ranking of feature importance for the preoperative prediction of PC-AKI, as generated by the RF model. The top 15 preoperative variables selected to establish Model 1, in order of importance, were urine protein, diuretics, myocardial infarction, diabetes, congestive heart failure, cardiac troponin T, β-blockers, NT-proBNP, hemoglobin, creatine kinase, arrhythmia, left ventricular ejection fraction (LVEF), creatine kinase-MB, albumin, calcium. Model 2 incorporated 5 additional intraoperative features: IABP, PCI, vasoactive drugs, contrast volumes, and emergency procedures.

Performance comparison of multiple ML methods applied to Model 1

Table 3 presents the performance of six ML algorithms for Model 1 on the validation cohort. Figure 4 illustrates the AUROC curve and the AUPRC curve of each model in the validation cohort. The DNN model achieved the highest AUROC of 0.733 (95% CI 0.654-0.812) and the highest AUPRC of 0.348. It was followed by the NB model, the LR model, the XGBoost model, the RF model, and the KNN model, ranked by predictive efficiency from high to low. The DNN model was finally selected as the preoperative predictive model for PC-AKI. Table 4 presents the predictive performance of the DNN model at its optimal cutoff value of 0.459. At this cutoff, the model exhibited a sensitivity of 70.3% and a specificity

Table 3. Performance of the six ML algorithms applied to Model 1 in the validation cohort.

	AUROC	AUPRC
DNN	0.733	0.348
NB	0.715	0.322
LR	0.687	0.308
KNN	0.648	0.241
RF	0.653	0.210
XGBoost	0.667	0.238

Abbreviations: AUROC, area under the receiver operator characteristic curve; AUPRC, area under the precision-recall curve; DNN, deep neural network; NB, naive Bayes; LR, logistic regression; KNN, k-nearest neighbors; RF, random forest; XGBoost, extreme gradient boosting.

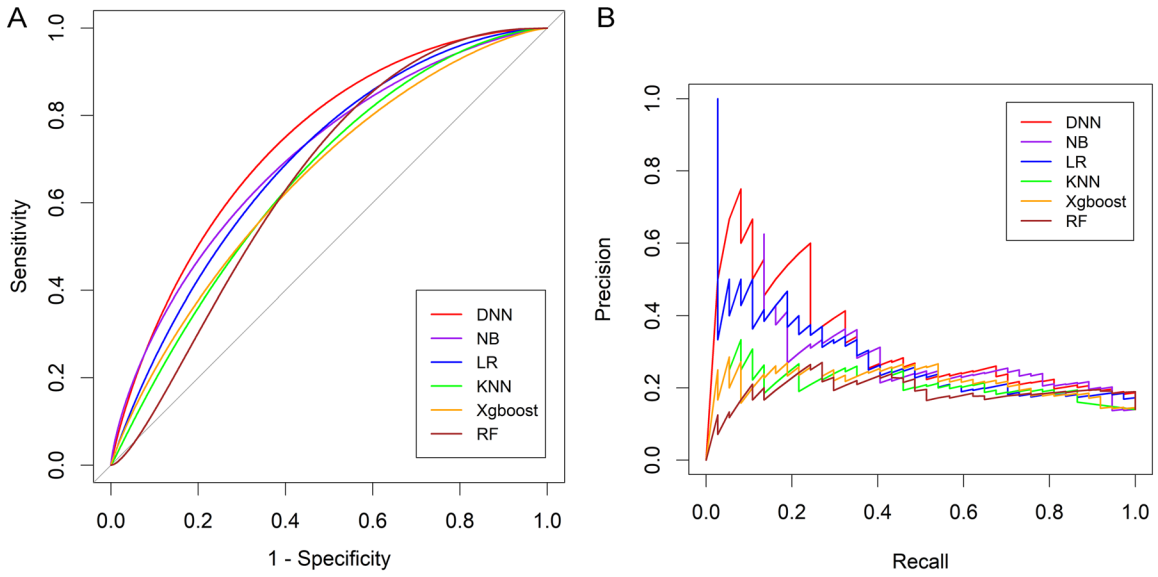

Figure 4. Receiver operating characteristic curves and precision-recall curves of the six ML algorithms applied to Model 1 in the validation cohort. Abbreviations: DNN, deep neural network; NB, naive Bayes; LR, logistic regression; KNN, k-nearest neighbors; XGBoost, extreme gradient boosting; RF, random Forest.

Table 4. Performance of the preoperative predictive model for PC-AKI based on the DNN algorithm.

	Derivation cohort	Validation cohort
Cutoff value	0.460	0.459
Sensitivity, %	82.1	70.3
Specificity, %	60.1	63.4
PPV, %	67.3	23.9
NPV, %	77.0	92.9
PLR	2.058	1.921
NLR	0.298	0.468

Abbreviations: PPV, positive predictive value; NPV, negative predictive value; PLR, positive likelihood ratio; NLR, negative likelihood ratio.

of 63.4% on the validation cohort. The decision curve analysis revealed that a clinical net benefit is attainable, with diagnostic thresholds ranging from 0.04 to 0.79 in the derivation cohort and from 0.03 to 0.51 in the validation cohort, facilitating clinical decision-making (Figure 5). In sensitivity analysis, the DNN model showed robust performance, with the AUROC being 0.732 in patients with eGFR < 45 mL/min/1.73 m^2 and 0.753 in those with eGFR ≥ 45 mL/min/1.73 m^2. When stratifying patient groups based on age, gender, and comorbidities, the performance of the model remained relatively stable (Supplementary Figure S1–4).

Performance comparison of multiple ML methods applied to Model 2

The performance of multiple ML methods for Model 2 in the validation cohort is shown in Table 5. The AUROC curve and the AUPRC curve of each model in the validation cohort are shown in Figure 6. The addition of intraoperative variables improved the performance of the DNN model, with the AUROC of 0.770 (95% CI 0.695-0.845) and the AUPRC of 0.415. It was followed by the NB model, the LR model, the RF model, the XGBoost model, and the KNN model, ranked by predictive efficiency from high to low. The Mehran score exhibited an AUROC of 0.631 (95% CI 0.538-0.724) and an AUPRC of 0.212. The DNN model was finally selected as the postoperative predictive model for PC-AKI. Table 6 presents the predictive performance of the DNN model at its optimal cutoff value of 0.456. With the incorporation of intraoperative variables, the DNN model achieved a sensitivity of 81.1% and a specificity of 61.7% on the validation cohort. The decision curve analysis revealed that a clinical net benefit is attainable, with diagnostic thresholds ranging from 0.05 to 0.92 in the derivation cohort and from 0.03 to 0.61 in the validation cohort, thereby supporting clinical decision-making (Figure 7). In sensitivity analysis, the DNN model showed robust performance, with the AUROC being 0.743 in patients with eGFR < 45 mL/min/1.73 m^2 and 0.778 in those with eGFR ≥ 45 mL/min/1.73 m^2 When stratifying patient groups based on age, gender, and comorbidities, the performance of the model remained relatively stable (Supplementary Figure S5–8).

Explanation of DNN models with the SHAP method

The SHAP method was used to present a comprehensive swarm plot to interpret the predictions of the DNN models (Figure 8). The SHAP swarm plot revealed that myocardial infarction, diabetes, higher urine protein level,

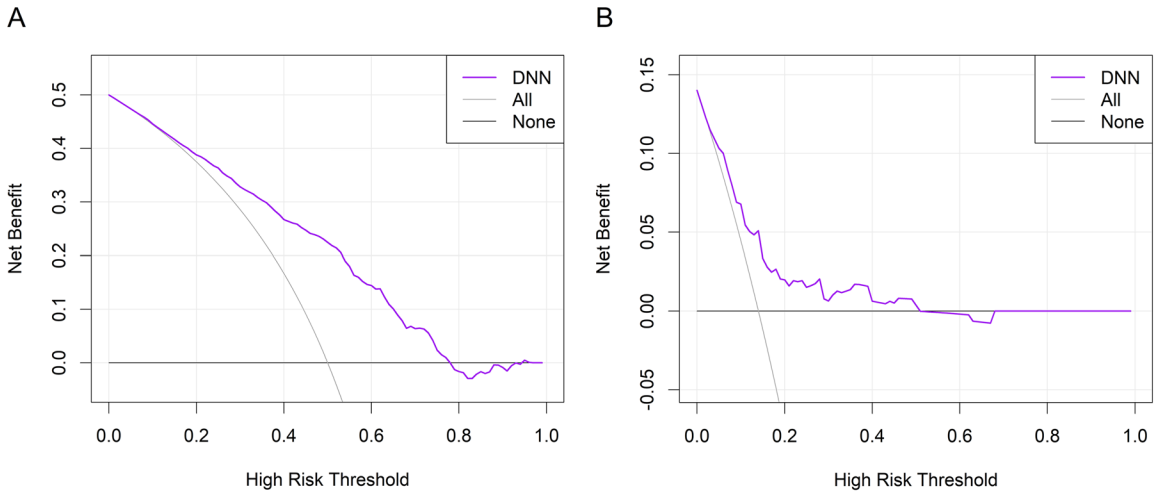

Figure 5. Decision curves of the preoperative predictive model for PC-AKI based on the DNN algorithm in the derivation cohort (A) and the validation cohort (B).

Table 5. Performance of the six ML algorithms applied to Model 2 in the validation cohort.

	AUROC	AUPRC
DNN	0.770	0.415
NB	0.713	0.334
LR	0.703	0.353
KNN	0.615	0.208
RF	0.682	0.255
XGBoost	0.674	0.253

Abbreviations: AUROC, area under the receiver operator characteristic curve; AUPRC, area under the precision-recall curve; DNN, deep neural network; NB, naive Bayes; LR, logistic regression; KNN, k-nearest neighbors; RF, random forest; XGBoost, extreme gradient boosting.

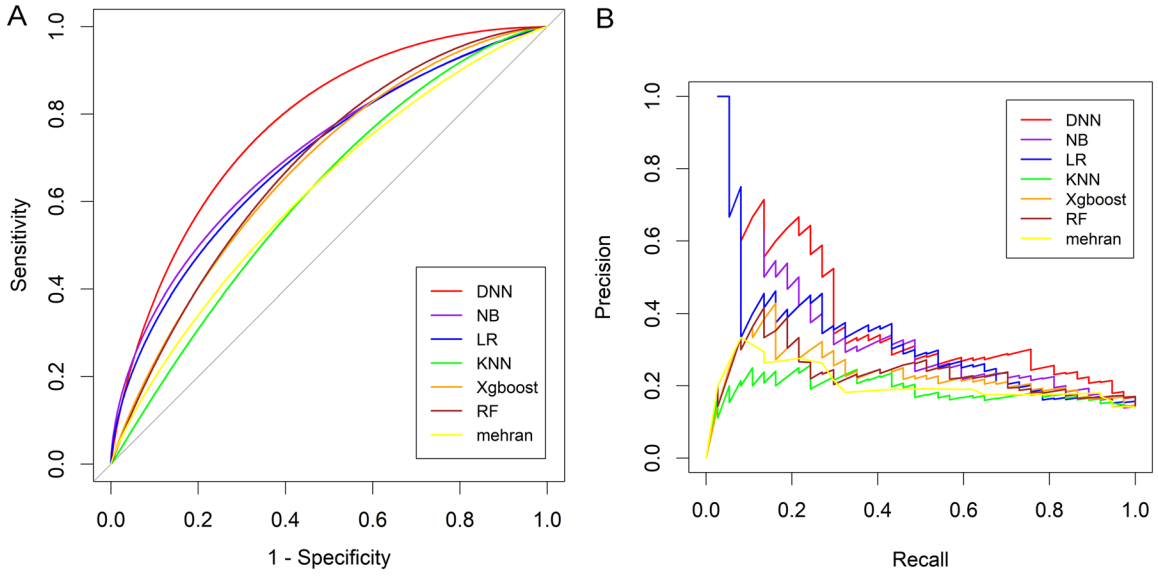

Figure 6. Receiver operating characteristic curves and precision-recall curves of the six ML algorithms and Mehran score applied to Model 2 in the validation cohort. Abbreviations: DNN, deep neural network; NB, naive Bayes; LR, logistic regression; KNN, k-nearest neighbors; XGBoost, extreme gradient boosting; RF, random Forest.

congestive heart failure, and lower hemoglobin level were the top five factors associated with increased risk of PC-AKI in Model1. While myocardial infarction, diabetes, higher urine protein level, PCI, and congestive heart failure were the top five factors associated with increased risk of PC-AKI in Model 2.

A web-based tool for PC-AKI

The DNN models for predicting PC-AKI were designed as a user-friendly web-based risk tool (https://xydsbakigroup.streamlit.app/). Details of the web-based tool can be found in Supplementary Figure S9.

Table 6. Performance of the postoperative predictive model for PC-AKI based on the DNN algorithm.

	Derivation cohort	Validation cohort
Cutoff value	0.456	0.456
Sensitivity, %	82.4	81.1
Specificity, %	60.4	61.7
PPV, %	67.6	25.6
NPV, %	77.5	95.2
PLR	2.081	2.117
NLR	0.291	0.306

Abbreviations: PPV, positive predictive value; NPV, negative predictive value; PLR, positive likelihood ratio; NLR, negative likelihood ratio.

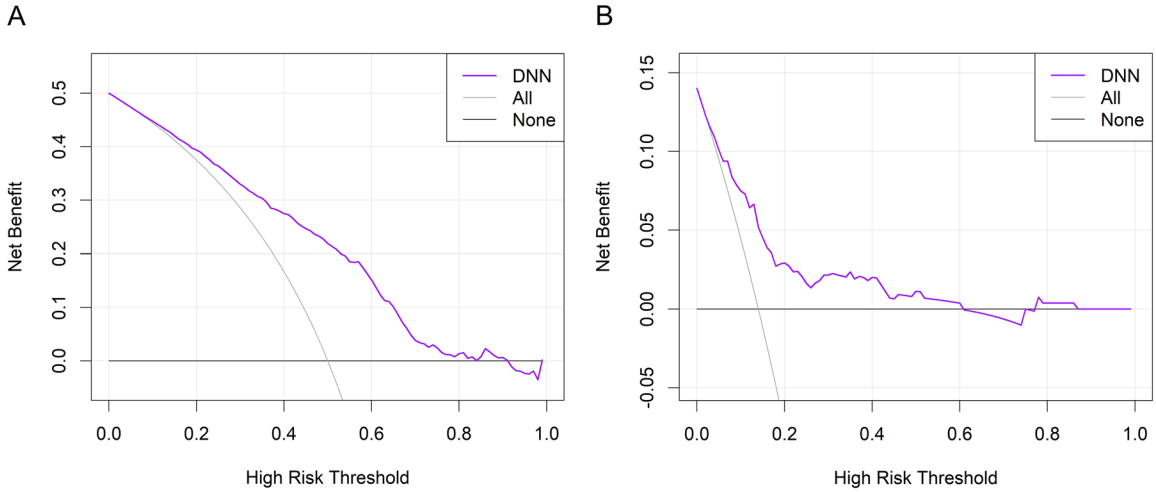

Figure 7. Decision curves of the postoperative predictive model for PC-AKI based on the DNN algorithm in the derivation cohort (A) and the validation cohort (B).

Discussion

The present study applied six ML algorithms to predict the risk of PC-AKI in CKD patients undergoing coronary angiography and intervention procedures. Among these, the DNN algorithm achieved the best predictive performance in the validation cohort. Two predictive models for PC-AKI were developed and validated: one based on 15 preoperative variables and the other incorporating an additional 5 intraoperative variables. The SHAP method enhanced the interpretability of the DNN models. We also developed a user-friendly web-based tool to facilitate their clinical application. These models have the potential to support clinical decision-making and early intervention by individualized risk assessment at two time points.

PC-AKI is a common and severe complication following the intravascular administration of iodinated contrast media [6–8]. Currently, the understanding of the development and prognosis of PC-AKI in CKD patients undergoing coronary angiography and intervention remains insufficient. Our previous study found that the incidence of PC-AKI ranged from 10.3% to 11.4% in hospitalized CKD patients receiving intravenous iodinated contrast media [23]. In this study, we further investigated the development and prognosis of PC-AKI in patients with CKD undergoing CAG or PCI. The incidence of PC-AKI after CAG/PCI in the CKD population was 12.8%, which is broadly consistent with the 12.1% reported by Maioli et al. and slightly lower than the 14.9% observed by Lei et al. [6,30]. In addition, our study indicated that the occurrence of PC-AKI was associated with an increased risk of MAKE30, as well as short-, mid-, and long-term mortality. PC-AKI is not merely a transient elevation in SCr but is closely linked to adverse outcomes, including worsening renal function, persistent renal insufficiency, dialysis, and death. This emphasizes the critical importance of early identification and prevention of PC-AKI.

The development of clinical prediction models to accurately predict PC-AKI in patients undergoing coronary angiography and intervention in an area of significant interest. Such models can help clinicians identify high-risk patients and implement early interventions. Several predictive models for PC-AKI following coronary angiography and intervention have been reported previously. Among these, the Mehran score is currently the most widely used model in clinical practice. Since its introduction in 2004, the Mehran score has undergone multiple external validations and is widely recognized for its reliability. In twelve external validation studies comprising 13,522 patients, the average weighted C-statistic for the Mehran score was 0.72 (95% CI 0.63-0.80), with high heterogeneity [17]. However, the performance of the Mehran score in specific populations still requires validation. In our study, the Mehran score exhibited a relatively low AUROC of 0.631 (95% CI 0.538-0.724) for predicting PC-AKI in a cohort of CKD patients, indicating limited predictive power.

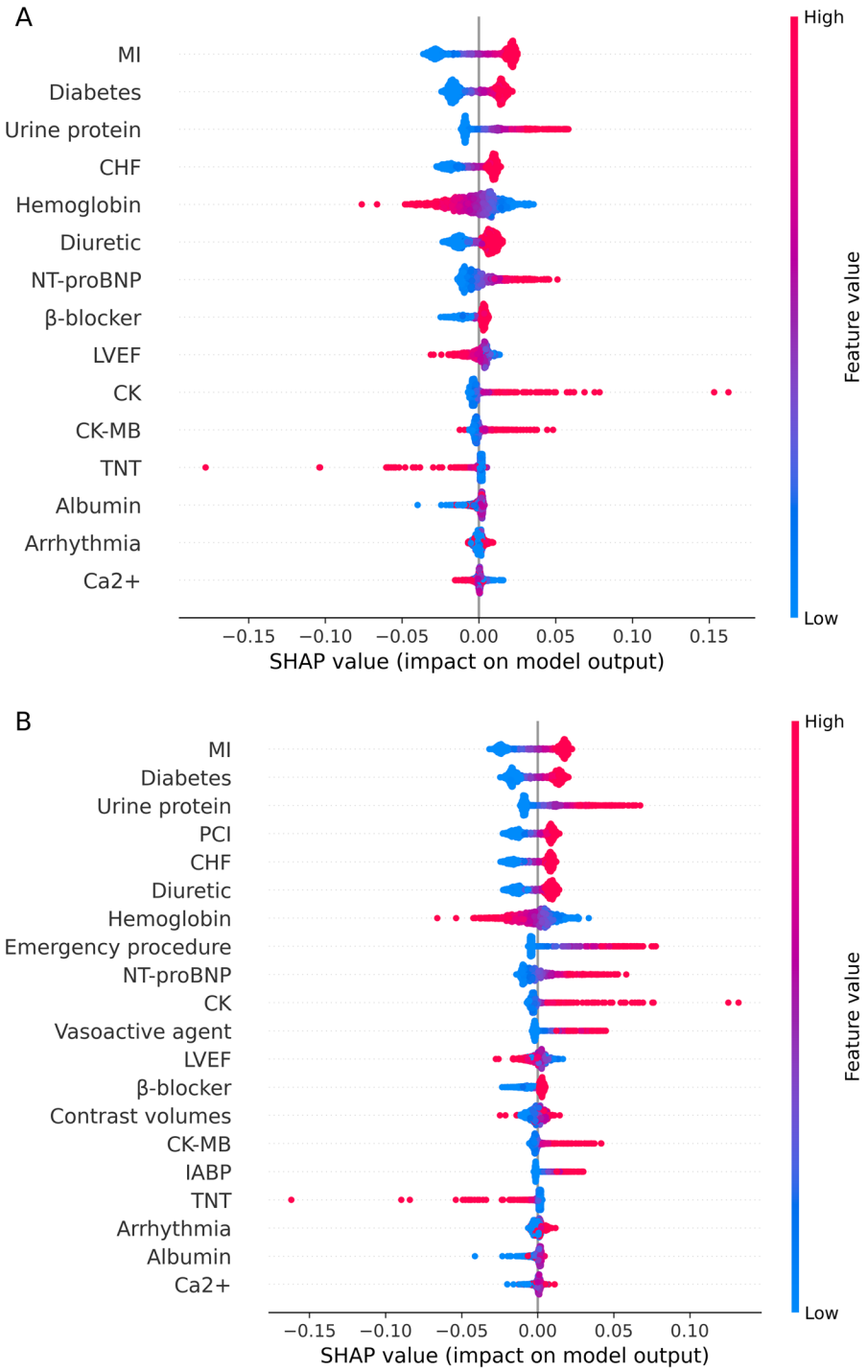

Figure 8. SHAP swarm plot of the DNN algorithm applied to Model 1 (A) and Model 2 (B). The horizontal axis represents the SHAP values, indicating the contribution of each feature to the model's predictions. Positive SHAP values suggest a positive contribution to the predicted outcome, while negative values indicate a negative contribution. The vertical axis lists the features, arranged in order of their overall importance based on average absolute SHAP values. Each point on the plot corresponds to an individual instance's SHAP value for a specific feature. Blue indicating lower values and red indicating higher values. Abbreviations: MI, myocardial infarction; CHF, congestive heart failure; NT-proBNP, N-terminal pro-B-type natriuretic peptide; LVEF, left ventricular ejection fraction; CK, creatine kinase; CK-MB, creatine kinase-MB; TNT, cardiac troponin T; PCI, percutaneous coronary intervention; IABP, intra-aortic balloon pump.

Additionally, the Mehran score incorporated intraoperative variables such as the use of IABP and the volume of contrast media, which makes it difficult to assess the risk of PC-AKI before the procedure. To minimize the risk of PC-AKI, it is crucial to determine the necessity of the procedure and implement preventive interventions beforehand. Brown et al. and Gurm et al. both stressed the need for preoperative risk assessment and the construction of predictive models using preoperative variables [38,39].

Renal insufficiency stands as one of the most important independent risk factors for PC-AKI. Patients with CKD are considered the primary population at risk for PC-AKI. This

group is also characterized by a high prevalence of coronary artery disease and a frequent need for coronary procedures for diagnosis and treatment [40,41]. Clinicians often face a dilemma when deciding whether to proceed with the procedures. At present, eGFR is a key criterion for identifying high-risk groups for PC-AKI, as recommended by the guidelines [10–12]. Compared to using eGFR alone, predictive models provide a more accurate identification of CKD patients who are truly at high risk for PC-AKI. However, there are few predictive models specifically developed for this group. Lei et al. developed a nomogram to predict PC-AKI in patients with CKD undergoing CAG or PCI[30]. Using multivariable logistic regression and a stepwise approach, six key predictors of PC-AKI were identified and incorporated into the nomogram: age, weight, heart rate, hypotension, PCI, and β-blocker use. The nomogram was internally validated using the bootstrap method, achieving an AUROC of 0.76. It demonstrated better predictive performance compared to the Mehran score that had an AUROC of 0.71. Nevertheless, the study was limited by the lack of external validation and a relatively small sample size. Additionally, using PCI as a predictor may not be suitable for preoperative risk assessment, as it is not always feasible to determine the need for PCI before the procedure.

Compared to previously reported models for PC-AKI, our study presents several advantages. Firstly, we employed six distinct ML methods to develop predictive models for PC-AKI and identified the DNN model as the best-performing one. The DNN algorithm excels at learning features from complex, multi-modal, and high-dimensional data, significantly enhancing prediction efficiency compared to traditional methods. This is consistent with our previous study, which utilized the DNN algorithm to develop a predictive model for PC-AKI in CKD patients receiving intravenous iodinated contrast media. The model demonstrated excellent predictive performance in both internal (AUROC 0.939) and external validation (AUROC 0.940) cohorts, outperforming the traditional logistic regression model [23].

Secondly, DNN models are often referred to as "black box" due to their complex multi-layer structure and large number of parameters, which make the decision-making process difficult to interpret and understand. In this study, we used explainable SHAP method to help healthcare providers understand how DNN models arrives at predictions, potentially increasing trust and adoption in clinical practice. Such transparency is essential for clinical decision-making and risk assessment.

Thirdly, the models were externally validated through temporal validation, employing a validation cohort comprised of patients admitted during different time periods within the entire study population [42]. The model exhibited good predictive performance in the validation cohort, highlighting its generalizability.

Finally, we developed two time-point risk predictive models that enable clinicians to assess patient conditions and support clinical decision-making. All of the predictor variables can be easily obtained in clinical settings. Model 1 incorporated only preoperative variables, providing an initial risk assessment to guide the selection of the procedure and the initiation of early interventions. Currently, saline hydration is the only evidence-based strategy proven effective in preventing PC-AKI, while the efficacy of pharmacological prophylaxis and preventive RRT remains unestablished [4,10]. Several studies have indicated that hydration guided by hemodynamic parameters is more effective than standard hydration protocols in reducing the risk of PC-AKI and improving patient outcomes [43–45]. Additionally, ultra-low contrast PCI and imaging- and physiology-guided PCI without contrast administration have been demonstrated to be feasible and safe [46,47]. These approaches provide a viable strategy for patients at high risk of PC-AKI to undergo CAG or PCI without adverse effects on residual renal function. Model 2 incorporated both preoperative and intraoperative variables, and the addition of intraoperative variables enhanced its discrimination and sensitivity compared to Model 1. This model offers more accurate predictions of PC-AKI and could advance a personalized, adaptive approach to patient care. It is critical to closely monitor renal function in high-risk patients postoperatively and to provide timely interventions if complications arise. To facilitate the clinical application of the models, we further developed a web-based risk tool that can automatically predict the risk of PC-AKI and provide management recommendations. This tool serves as a decision-making support system for clinicians.

However, this study is also subject to several limitations. Firstly, it is a single-center retrospective study, which limits the generalizability of our findings to other healthcare settings and populations. Secondly, the sample size in this study is relatively small, especially for deep learning applications which typically require large datasets to achieve optimal performance. Thirdly, the temporal validation approach used in this study was limited to patients from 2021. A more comprehensive validation strategy, including longer validation periods and external validation from different time periods, would provide a more robust assessment of the model's stability and performance over time. Fourthly, the web-based tool presented in this study offers significant potential for enhancing clinical practice, yet its validation in real-world clinical settings is still needed. Moreover, the study's impact on clinical decision-making and patient outcomes remains unclear. Finally, even with random forest imputation to handle missing values, additional bias may still be introduced, potentially compromising the accuracy of predictive models. Future research should further validate the model and tool's generalizability and clinical efficiency in larger, multi-center patient cohorts.

Conclusion

This study developed and validated two DNN-based models to predict PC-AKI in CKD patients undergoing coronary angiography and intervention procedures. Model 1 incorporates preoperative variables for preoperative risk assessment, while

Model 2 includes additional intraoperative variables for post-operative evaluation. The SHAP method provided interpretability for the DNN models, which improved the transparency of the clinical decision-making process. A user-friendly web-based risk tool was developed that serves as a promising tools for risk assessment and clinical decision-making.

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Not applicable.

Author contributions

SD and XL designed and supervised the study and revised the manuscript. YT performed the data extraction, analyzed and interpreted the data and drafted the manuscript. TW, XW, XW, YL and MZ interpreted the data and critically revised the manuscript. AC, GC, CT and LH performed the data extraction and revised the manuscript critically for important intellectual content. All authors read and approved the final manuscript.

Disclosure statement

No potential conflict of interest was reported by the author(s).

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Data availability statement

The data and source codes utilized in this study are accessible from the corresponding author upon reasonable request.

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