

Prediction of dialysis adequacy using data-driven machine learning algorithms

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ABSTRACT

Background: Adequate delivery of hemodialysis (HD), measured by the spKt/V derived from urea reduction, is an important determinant of clinical outcomes in chronic hemodialysis patients. However, the need for pre- and postdialysis blood samples prevented the assessment of spKt/V in every session.

Methods: This retrospective single-center study was performed on end-stage renal disease (ESKD) patients aged ≥ 18 years who received standard thrice-weekly chronic HD therapy. Eighty-seven variables, including general, intradialytic, and laboratory variables, were collected from the medical records for analysis. Five steps of preprocessing procedure were deployed to select only the most relevant variables. Six binary classification models were developed to predict whether spKt/V was higher than 1.4.

Results: A total of 1869 HD sessions from 373 ESKD patients were included in this study. The Random Forest model showed the best prediction for dialysis adequacy, with AUROC scores of 0.860 in the validation dataset and 0.873 in the testing dataset. Notably, an accessible model that solely relied on noninvasively collected general and dialysis-related variables maintained high prediction accuracy, with AUROC scores of 0.854 and 0.868 in the validation and testing datasets, respectively. The five most significant predictive variables were vascular access, gender, body mass index, ultrafiltration volume, and dialysis duration.

Conclusion: The study results suggest that the development of ML models for accurately predicting dialysis adequacy based on general and intradialytic variables is feasible. These models have the potential to be utilized for noninvasive clinical assessments of dialysis adequacy.

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Introduction

Adequate dialysis treatment is a crucial factor determining the survival outcomes of end-stage kidney disease (ESKD) patients receiving hemodialysis (HD) [1]. The single-pool Kt/V (spKt/V; K , urea dialytic clearance; t , dialysis time; V , urea distribution volume) is a widely used measurement for evaluating dialysis adequacy, which represents the clearance of small molecular weight molecules in an HD session [2]. Recent guidelines recommend a spKt/V of 1.4 per HD session for patients undergoing thrice-weekly treatment [3]. However, the spKt/V has several limitations. Given that it requires invasive blood sampling both before and after HD, assessing the spKt/V in every session is impractical, imposing significant financial burdens on both patients and healthcare providers [4]. Currently, the spKt/V is recommended to be measured at

least once per month, with the implicit assumption that one HD session could represent of all sessions in a certain period [3]. However, the spKt/V evaluated during a single HD session may fail to capture potential inadequate dialysis in other sessions due to variations in numerous parameters across different sessions [1]. Therefore, a model that has the ability to predict the dialysis adequacy in a less invasive way is needed to reduce financial burden and blood exposure but also improve survival rates.

Reports have shown that demographic, dialytic, and laboratory variables are related to dialysis adequacy [5,6]. Progresses have been made in identifying these factors; however, utilizing them in predicting dialysis adequacy may be impractical as those factors are too complex to be processed manually [4]. Currently, no predictive models based on logistic regression have been established in clinical practice.

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Machine learning (ML) is emerging as the best solution for dealing with vast and complex medical data [7]. Compared with manual feature extraction, machine learning is capable of capturing both linear and nonlinear relationships and patterns within high-dimensional data in an automatic way. In recent years, ML has been applied in the healthcare field to construct prediction models for a variety of diseases, such as gestational diabetes mellitus, acute kidney injury, and intradialytic hypotension [8,9]. However, application in predicting the dialysis adequacy is lacking.

In this study, we hypothesized that ML algorithms have the ability to predict the dialysis adequacy. To this end, we aimed to build ML models to predict whether spKt/V is higher than 1.4, based on demographic, intradialytic, and laboratory variables.

Methods

Study population

This study included all end-stage renal disease patients aged ≥ 18 years who received standard thrice-weekly chronic hemodialysis therapy for at least 6 months at Chongming Center Hospital Affiliated to Shanghai University of Medicine & Health Sciences (CCH). Data were collected retrospectively from January 2023 and December 2023 and prospectively from January 2024 and May 2024. The institutional review boards waived the requirement for written informed consent for patients included in the retrospective cohort, while written informed consent was obtained from every patient in the prospective cohort. To comply with Transparent Reporting of a Multivariable Prediction Model for Individual Prognosis or Diagnosis (TRIPOD) guidelines, patients retrospectively collected between January 2023 and December 2023 were randomly split into a training data set and a validation data set with a fixed ratio of 7:3. Patients prospectively recruited between January 2024 and May 2024 comprised the testing set. The following were the exclusion criteria: (1) patients without a stable, functioning arteriovenous access; (2) patients without satisfactory compliance with HD treatment (i.e., patients who missed more than 15% of their scheduled dialysis sessions over a 3-month period, or patients who failed to adhere to fluid restrictions, necessitating additional HD sessions); (3) patients with a history of kidney transplantation; (4) patients with life-threatening conditions within six months before data collection; (5) patients with active systemic inflammatory disease (e.g., patients with systemic lupus erythematosus or rheumatoid arthritis showing active evidence, such as a fever higher than 38°C , joint pain and swelling, or rashes).

Outcomes

Adequate dialysis was defined as an spKt/V value of ≥ 1.4 for HD sessions of patients undergoing HD thrice weekly. Conversely, inadequate dialysis was defined as an spKt/V value less than 1.4 for the same population. The linear equation for spKt/V calculation follows The National Kidney

Foundation's Kidney Disease Outcomes Quality Initiative (KDOQI) guidelines [3]:

$$\text{spKt} / V = -\ln(R - 0.008 \times T) + (4 - 3.5 \times R) \times 0.55 \times \text{Weight loss} / V$$

where R is the ratio of postdialysis to predialysis BUN; V is the body water volume; Weight loss is expressed in the same units as V; and T is treatment time in hours. The predialysis blood samples were obtained before dialysis while postdialysis blood samples were acquired at the end of dialysis using a slow-flow method. All samples were collected during mid-week dialysis session.

Predictive features and data preprocessing

A total of 87 variables were considered for selection. They could be divided into three categories: (1) general information (e.g., age, predialysis body mass index (BMI)); (2) dialysis-related variables (e.g., dialysis vintage, vascular access, dialysis mode, intradialytic heart rate (HR), intradialytic blood pressure (BP)); and (3) laboratory variables gathered from predialysis blood samples (e.g., hemoglobin, triglyceride). Intradialytic BP and HR were measured every hour from the start of each session. The median number of BP and HR recordings obtained during dialysis was four (range: 3–4). We therefore calculated average value (AVR), standard deviation (SD), and coefficient of variation (CV) of intradialytic BP and HR. Considering the source of each variable, we extracted general information and dialytic variables to create an “easy-to-use” set, as these data could be conveniently obtained with minimal financial cost.

To make the origin data suitable machine learning algorithms, we applied the following data pro-processing procedures to both all variables and ‘easy-to-use’ variables. Firstly, variables with more than 20% missing values were excluded. Secondly, Multiple Imputation by Chained Equations (MICE) algorithm was applied to impute the missing data by predictive mean matching [10]. To avoid data leakage, the imputation for training and testing datasets was done separately. We imputed the continuous variables using ‘mean’ strategy and ‘most frequent’ for the categorical variables. Thirdly, continuous variables were normalized using Z-score normalization. Finally, collinearity was detected by calculating the variance inflation factor (VIF). Variables were removed one by one until all variables had VIFs lower than five.

Model construction

Six models were included to predict whether spKt/V is higher than 1.4 or not: logistic regression (LR), decision tree (DT), random forest (RF), support vector machine (SVM), adaptive boosting (Adaboost), and extreme gradient boosting (Xgboost). With the training data set, hyper-parameters of each model were optimized by grid search using 10-fold nested cross-validation. During hyper-parameters optimization, a range of values for each hyperparameter was specified, and all combinations of these values are tested. For each combination, the model's performance was evaluated

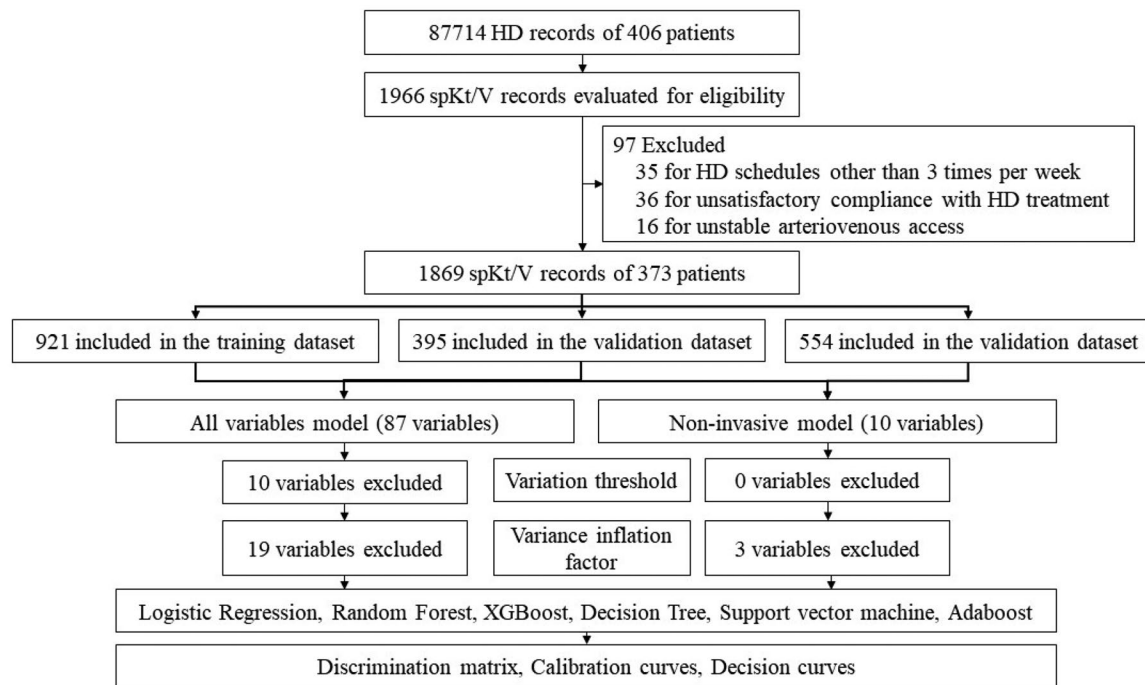


Figure 1. Flowchart showing an overview of the machine learning approach.

using 10-fold cross-validation and the hyperparameter combination that yields the best accuracy was selected as the optimal set of hyperparameters for the final model. The range of values of each hyper-parameter were listed in [Supplementary Table S1](#). We compared the models in terms of discrimination and calibration. The discrimination was measured by the accuracy, sensitivity, specificity, positive predictive value (PPV), negative predictive value (NPV), and the area under the receiver operating characteristic curve (AUROC). The calibration was assessed visually using calibration plots and measured quantitatively by brier score. The AUROC was used as a standard performance metric to optimize the models. Decision curve analysis was used to calculate the net benefit for potential clinical use.

Statistical analysis

The descriptive statistics are done using ‘SCIPY’ package of Python language. Continuous variables were presented as mean \pm standard deviation or as the median (quartile [Q] 25–Q75) if the data were not normally distributed. Categorical variables were presented as number (%) and compared using the χ^2 tests or Fisher exact tests. Continuous variables were compared using *t*-tests or Mann–Whitney U-test if the data were not normally distributed. All analyses were performed using Python, version 3.11.7.

Results

Database description and preprocessing

The database contained a total of 87714HD records of 406 patients. Screening for those patients with spKt/V recordings

revealed 1869HD sessions of 373 patients. Comparisons of the variable characteristics between the training, the validation and the testing datasets are presented in [Supplementary Table S2](#).

The overall workflow pattern of this study is shown in [Figure 1](#). Firstly, we evaluated the missing value of each variable and variables with more than 20% missing value were removed ([Supplementary Figure S1](#)). [Supplementary Figure S2](#) shows the distribution of all continuous variables for extreme outliers checking. All extreme outliers were kept because they were collected in real clinical situations. Variables with near-zero variance and were removed, which were prealbumin, Albumin/Globulin ratio, uric acid, Ca, Mg, platelet crit, basophil ratio, monocytes count, eosinophils count, and basophils count. Multiple imputations were applied to thirty-nine variables with missing value. The sensitivity analysis showed no difference in the missing data before and after imputation ([Supplementary Table S3](#)). The results of collinearity analysis suggested that forty-eight variables were included for the final model as they had VIFs lower than five ([Supplementary Table S4](#)).

Models predicting dialysis adequacy based on all variables

The discrimination results of six different classification models to predict dialysis adequacy on both validation and testing datasets were listed in [Table 1](#). The fine-tuned hyper-parameters for each model were listed in [Supplementary Table S1](#). The RF model demonstrated the best discrimination in both the validation dataset (AUROC = 0.860, [Figure 2\(a\)](#)) and the testing dataset (AUROC = 0.873, [Figure 2\(b\)](#)). The model diagnostics for this best performing model were shown in [Supplementary Figures S3 and S4](#). The decision curve analysis indicated that when the threshold probability

Table 1. Discrimination metrics of each ML model predicting the dialysis adequacy.

Models	The validation dataset						The testing dataset					
	Accuracy	Sensitivity	Specificity	PPV	NPV	AUROC	Accuracy	Sensitivity	Specificity	PPV	NPV	AUROC
All variables												
LR	0.825	0.558	0.921	0.716	0.854	0.849	0.837	0.587	0.924	0.730	0.865	0.868
RF	0.828	0.481	0.952	0.781	0.837	0.860	0.846	0.601	0.932	0.754	0.870	0.873
SVM	0.808	0.529	0.907	0.671	0.843	0.801	0.797	0.622	0.859	0.605	0.867	0.835
XGBoost	0.818	0.519	0.924	0.711	0.843	0.855	0.819	0.636	0.883	0.655	0.874	0.844
DT	0.790	0.317	0.959	0.733	0.797	0.637	0.794	0.776	0.8	0.575	0.911	0.787
Adaboost	0.808	0.500	0.918	0.684	0.837	0.828	0.819	0.580	0.902	0.675	0.860	0.775
Easy-to-use variables ^a												
LR	0.810	0.452	0.938	0.723	0.827	0.854	0.843	0.559	0.941	0.769	0.860	0.868
RF	0.813	0.519	0.918	0.692	0.842	0.841	0.814	0.706	0.851	0.623	0.893	0.864
SVM	0.823	0.596	0.904	0.689	0.862	0.844	0.830	0.713	0.871	0.658	0.897	0.867
XGBoost	0.803	0.538	0.897	0.651	0.845	0.826	0.812	0.601	0.885	0.647	0.864	0.860
DT	0.810	0.519	0.914	0.684	0.842	0.812	0.846	0.594	0.934	0.759	0.868	0.839
Adaboost	0.818	0.490	0.935	0.729	0.837	0.844	0.835	0.622	0.910	0.706	0.874	0.851

AUROC: area under the receiver operating characteristic curve; Adaboost: adaptive boosting; DT: decision tree; LR: logistic regression; RF: random forest; SVM: support vector machine; XGBoost: extreme gradient boosting.

^aeasy-to-use variables included general and dialytic variables, both of which are collected noninvasively with minimal financial cost.

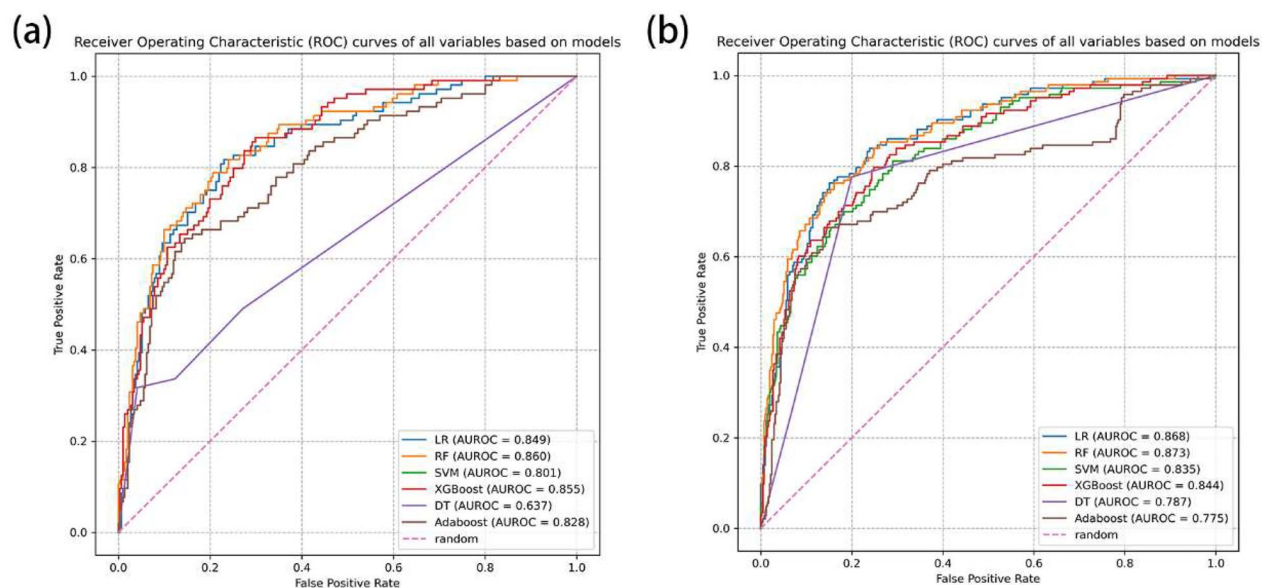


Figure 2. Model performance for each model based on all variables predicting dialysis adequacy. (a) the receiver operating characteristic (ROC) curve of each model, using all variables, based on the validation dataset; (b) the ROC of curve of each model, using all variables, based on the testing dataset. LR: logistic regression; RF: random forest; DT: decision tree; SVM: support vector machine (SVM), Adaboost: adaptive boosting; XGboost: extreme gradient boosting; AUROC: the area under the receiver operating characteristic curve.

was below 0.89, the net benefit of the RF model based on all variables was higher than both the 'intervention for all' and 'intervention for none' strategies (Supplementary Figure S3). Similarly, when the threshold probability was below 0.91, the net benefit of the RF model based on easy-to-use variables exceeded both the 'intervention for all' and 'intervention for none' strategies (Supplementary Figure S4).

Models predicting dialysis adequacy based on easy-to-use variables

Six classification models based on noninvasive variables were compared (Table 1). The LR model demonstrated the best discrimination in both the validation dataset (AUROC = 0.854, Figure 3(a)) and the testing dataset (AUROC = 0.868, Figure

3(b)). The model diagnostics for this best performing model are shown in Supplementary Figures S5 and S6. The decision curve analysis showed that when the threshold probability was below 0.91, the net benefit of the model was higher than both the 'intervention for all' and 'intervention for none' strategies (Supplementary Figure S5). When the threshold probability was below 0.72, or between 0.74 and 0.83, the net benefit of the LR model based on easy-to-use variables was higher than both the 'intervention for all' and 'intervention for none' strategies (Supplementary Figure S6).

Variable importance

The importance of variables for predicting dialysis adequacy are shown in descending order (Supplementary Figure S7).

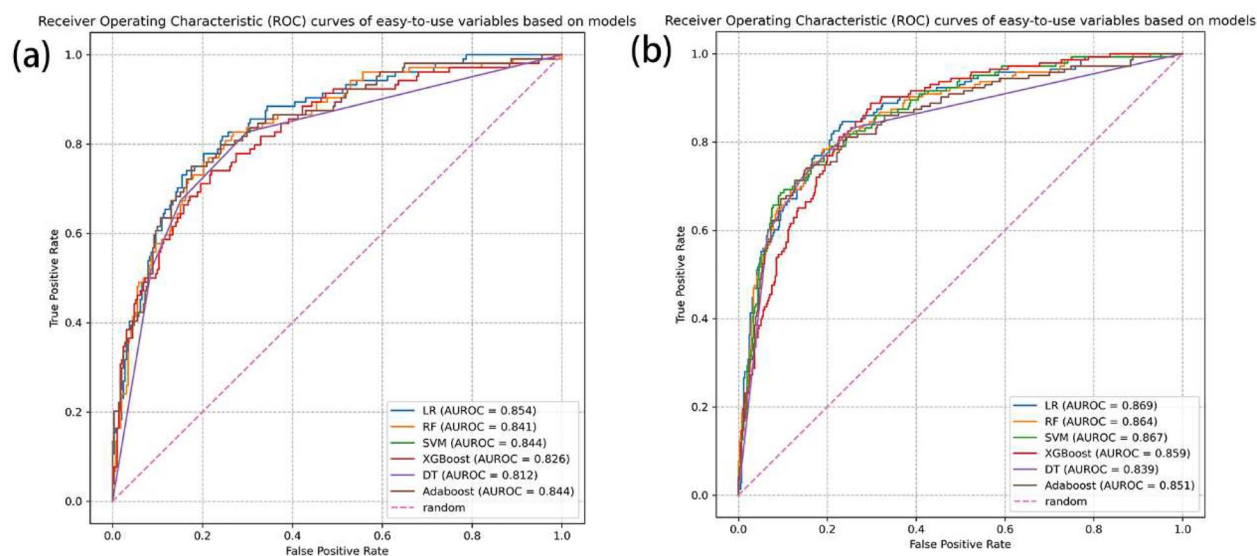


Figure 3. Model performance for each model based on all variables predicting dialysis adequacy. (a) the receiver operating characteristic (ROC) curve of each model, using easy-to-use variables, based on the validation dataset; (b) the ROC of curve of each model, using easy-to-use variables, based on the testing dataset.

LR: logistic regression; RF: random forest; DT: decision tree; SVM: support vector machine (SVM), Adaboost: adaptive boosting; XGboost: extreme gradient boosting; AUROC: the area under the receiver operating characteristic curve.

For both SHAP value of XGBoost model and feature importance of RF, the two most important variables based on all variables were gender and BMI. [Supplementary Figure S8a](#) displayed the SHAP value for a specific patient, indicating the contribution of each feature to the prediction result for that sample. Positive values indicate that the feature pushes the model output higher, while negative values indicate that the feature pushes the model output lower. [Supplementary Figure S8b](#) illustrated the SHAP summary plot for the entire test dataset. The horizontal axis displays samples ordered by similarity, and the vertical axis shows the model output $f(x)$. Each point's color represents the feature value (red indicates high values, blue indicates low values).

Discussion

In this study, we described for the first time a structured data-driven methodology to predict dialysis adequacy. Our findings in this study suggest that ML model has the ability to predict the dialysis adequacy with an AUROC of 0.874 based on general, dialytic, and laboratory variables. More interestingly, the exclusion of laboratory variables in the ML model did not lead to a notable decrease in performance.

Adequate dialysis is an important determinant of clinical outcomes in ESKD patients on HD. Many factors have been reported to be associated with dialysis adequacy, including gender, chemokines, and pre-dialysis weight [11,12]. However, no classification model has been adopted in clinical practice to predict dialysis adequacy because the relationship between clinical features and dialysis adequacy is too complex to be evaluated manually. The RF model that integrated general, dialytic, and laboratory variables achieved the best performance (0.873) in both the validation and testing sets,

while the LR model showed similar predictive performance (0.868) when based on easy-to-use features. The similarity in performance between RF and LR can be attributed to their respective strengths in handling different feature sets. Logistic regression, as a linear model, excels with fewer features by capturing the most significant relationships without the risk of overfitting. This allows it to deliver competitive results even with a simpler feature set. On the other hand, random forest, being a nonlinear model, thrives when provided with a larger number of features, enabling it to uncover complex interactions and patterns. The fact that logistic regression achieved comparable performance with a reduced number of features highlights its effectiveness in processing simpler datasets, while random forest's superior performance with a more extensive feature set showcases its capability to manage complex data structures. Using a well-calibrated, easy-to-use model can help physicians more accurately assess dialysis adequacy, optimize patient treatment plans, and improve overall treatment outcomes. The decision curve demonstrated that our model had a higher net benefit compared to an 'intervention for all' and an 'intervention for none'. All these findings indicate that our model provides nephrologists with a relatively precise dialysis adequacy assessment in every HD session.

One of the challenges in performing spKt/V assessment for every HD session is the need for pre- and post-dialysis collection of blood samples. Current guidelines recommend checking dialysis adequacy once per month, but the Kt/V assessed in one HD session does not account for potential inadequate dialysis doses that may be delivered during other sessions [3]. Our model based on all variables spares the need of postdialysis blood sampling, but still requires predialysis blood sample to function. Therefore, we further

described a simpler model only based on general and dialytic variables, both of which are collected noninvasively with minimal financial cost. An interesting finding was that the discriminative performance of models based on general and dialytic variables was similar to that of the model based on all variables. A possible explanation for this similarity may be that the variables that contributed most to the prediction are general variables. Previous studies have also reached similar conclusions. Several previous observational studies have revealed that women tend to have better dialysis adequacy and higher survival rates on dialysis compared to men [13]. This could be attributed to differences in body composition, hormonal influences, and perhaps even compliance with treatment and dietary recommendations. Women generally have a higher percentage of body fat and lower muscle mass compared to men, which may affect the distribution and clearance of urea during dialysis, potentially resulting in different adequacy levels [14]. The previous studies also found that higher BMI is often associated with lower dialysis adequacy [15]. This relationship might be due to the larger body size requiring a higher dialysis dose to achieve the same level of solute clearance. Excess adipose tissue can alter fluid distribution and increase peritoneal membrane transport rates, leading to less efficient waste removal.

Although some ML models for predicting the risk of acute kidney injury and dialysis control have been published, evidence for predicting dialysis adequacy is still lacking [9,16]. Kim and his colleagues established a number of regression models to predict the level of the urea reduction ratio (URR) using clinical demographics and repeated measurements [4]. In comparison with his study, our work employed classification algorithms, rather than regression algorithms, to predict dialysis adequacy. Furthermore, unlike his study that utilizes URR to evaluate dialysis adequacy, our article employs spKt/V for the same purpose, as it is recommended by current guidelines.

Our study has some limitations. First, although a relatively larger number of HD session and patients were included, we were unable to assess model generalizability in an external validation set. A large, prospective dataset is needed to evaluate the robustness of our model. The second is that some cytokines and chemokines related to dialysis adequacy were not included [11]. Although these features have been proved to be associated with dialysis adequacy prediction, their impact on ML performance remains unknown.

In conclusion, we developed ML prediction models that achieved good performance in predicting dialysis adequacy, both based on all variables and on easy-to-use variables alone. Vascular access, gender, BMI, ultrafiltration volume, and dialysis time were considered the most important predicting variables. Such models could be used for the clinical assessments of dialysis adequacy.

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Authors' contributions

L.Y.C. and X.L.X. contributed to the study design, methodology, and wrote the initial manuscript. L.Y.C., Q.J.P. and L.R. contributed to the data collection, analyzed and interpreted the data. C.J., X.L.X. and L.Y.C. contributed to the study figures and Tables. All authors reviewed the manuscript and approved the publication.

Disclosure statement

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Data availability statement

The data underlying this article will be shared on reasonable request to the corresponding author.

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