

- Hyper-parameters tuning for each ML algorithm using grid search and 10-fold cross-validation (final configuration of hyper-parameters for each ML algorithm is shown in Supplemental File 1)
- For K = 1 to 10:
 - Randomly divide the dataset into 5 folds with approximately equal sample size
 - For J = 1 to 5 (5-fold cross-validation):
 - ◆ Choose the J_{th} fold as validation set and the remaining four folds as training set
 - ◆ Develop four ML models (XGBoost, RF, DNN and LR) using the training set
 - ◆ Calculate AUC (AUC₀) for each ML model using the validation set
 - ◆ For I = 1 to 10:
 - ◇ Permute the values of the I_{th} variable in the testing set and calculate the corresponding AUC (AUC_i) for each ML model
 - ◇ Calculate AUC decrease for the I_{th} variable for each ML model: $1 - \frac{AUC_i}{AUC_0}$
- Calculate the mean decrease in AUC for each variable and each ML algorithm
- Ranking each variable in the four ML algorithms according to their mean decrease in AUC