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ML-based predictive model for adfreezing behavior of frozen soil-structure interface

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ABSTRACT

The punch shear test has been previously validated as a reliable method for estimating the adfreezing strength of the frozen soil-structure interface under unconfined conditions. Building upon this experimental research, the current study focuses on the development of four different machine-learning models (support vector machine (SVM), feedforward neural network (FNN), random forest (RF), and extreme gradient boosting (XGB)) to predict the adfreezing behavior using the experimental dataset. Among these models, the XGB model demonstrated the highest performance. Leveraging the results obtained from the XGB model, two post hoc analysis techniques were employed: prediction regions to assess prediction uncertainty and SHAP values to estimate the influence of input factors. In addition, the developed model's interpolation and extrapolation capabilities were evaluated. It was observed that the XGB model provided reasonable predictions within the limited range of the trained data, but yielded irrational values outside this range, thereby demonstrating the limitations of the data-based approach.

1. INTRODUCTION

In a previous study (Park 2022), the punch shear test was validated as a reliable method to estimate the adfreezing strength of the frozen soil-structure interface under unconfined conditions. During the ground's freeze-thaw process, adfreezing bond forms due to ice cementation at the interface between the frozen soil and structure, which can significantly impact the structure's stability in unexpected ways. Traditionally, the direct shear test has been used to investigate this adfreezing behavior by applying normal stress (Liu 2014; Wang 2019; Peng-Fei 2021). However, the punch shear test was proposed as an alternative, eliminating the need for additional assumptions in the direct shear test such as the direct assessment of the adfreezing strength under zero

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Machine learning (ML)-based predictive modeling, capable of building data-driven models without any assumptions, has shown excellent performance in predicting complex and nonlinear systems, and has been widely applied in various geotechnical studies (Fang 2018; Kim 2021; Pham 2021). However, ML models solely depend on given data, without considering physical information from previous studies, and their black box nature makes the interpretation of output results challenging, necessitating additional efforts to improve interpretability.

In this study, ML-based predictive models were developed to predict the adfreezing behavior at the interface between the frozen soil and structure under various conditions obtained from the punch shear test. The predictive performance of the models was compared, and the model with the best performance was subjected to analysis using two post-hoc methods.

2. DATABASE

The database involving 24 experimental cases consists of seven features for three soil specimens: displacement, adfreezing stress, mass median diameter (D_{50}), temperature, initial water content, unfrozen water content, and structural material (i.e., concrete and steel). The concrete structure conditions account for 81% of the total experimental data, while the steel structure conditions make up the remaining 19%. Since the structural material feature was in a categorical format, unsuitable for ML models, it was transformed into a numerical format using one-hot encoding.

Fig. 1 shows the Pearson correlation, which quantifies the linear relationship between two continuous variables ranging from -1 to 1. D_{50} showed negative correlations of about 0.65 with initial water content and unfrozen water content, while the correlation between initial water content and unfrozen water content was high at 0.98. The structural condition (concrete or steel) exhibited a complete negative linear relationship of -1 between the two features. Other relationships were found to be insignificant.

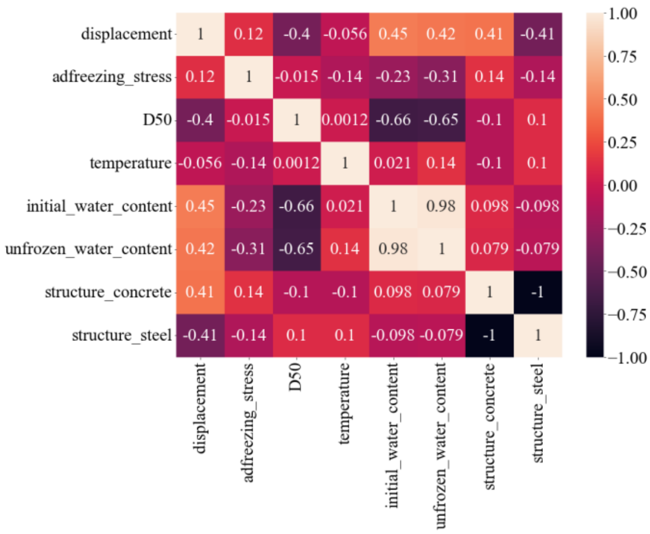


Fig. 1 Pearson correlation of features

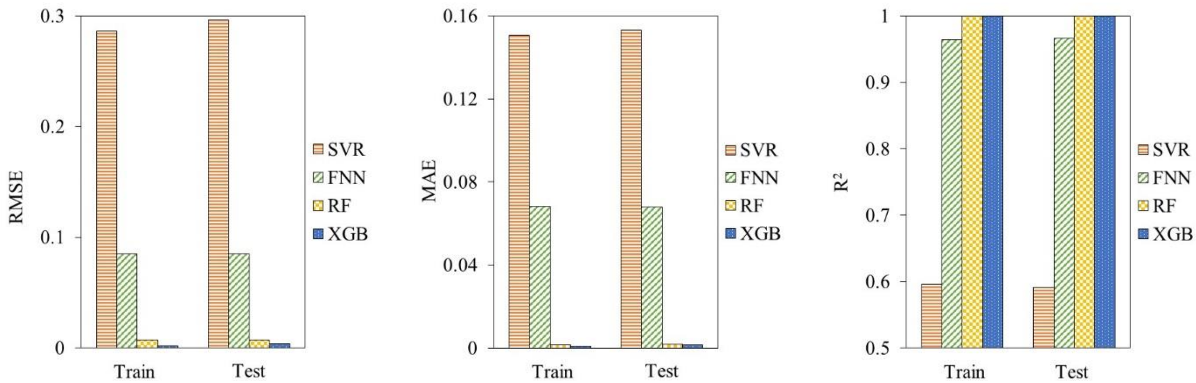
3. MODEL DEVELOPMENT

Four ML algorithms were employed to predict adfreezing behavior: support vector regression (SVR), feedforward neural network (FNN) with a single hidden layer, random forest (RF), and extreme gradient boosting (XGB). While the single models (SVR and FNN) have relatively simple structures, the ensemble models based on the decision tree model (RF and XGB) have more complex structures. In order to predict adfreezing stress as the target feature, the other six features were used as input factors. The database was divided into 70% for model training and 30% for model testing after standardizing the input data. To address data imbalance between steel and concrete structure conditions, a stratified random sampling technique was adopted for the training and testing datasets.

During the model training process, Bayesian optimization and five-fold cross-validation methods were employed to find hyperparameter combinations that offer the best performance. After the completion of hyperparameter tunning, the ML models were evaluated by three criteria: root mean squared error (RMSE), mean absolute error (MAE), and coefficient of determination (R^2).

4. REASULTS AND COMPARISON

Fig. 2 shows the prediction performances of the ML models. It can be observed that all models demonstrated higher prediction accuracy on the training data compared to the test data. In addition, ensemble models with relatively more complex structures outperformed single models on both the training and testing data. Among them, the XGB model showed the best performance.



(a) RMSE (b) MAE (c) R^2

Fig. 2 Performance comparison

Subsequently, the prediction uncertainty of the best-performing XGB model was explored by calculating the prediction interval. The prediction interval provides upper and lower prediction bounds with a certain confidence level. Notably, the calculated prediction interval of the XGB model included 98.42% of actual data at a 95% confidence level, emphasizing its reliability.

To estimate the influence of input features on adfreezing stress prediction, SHAP values of input factors were computed for the XGB model, as shown in Fig. 3. The SHAP analysis, based on the cooperative game theory, assigns an influence score to each predictor for the prediction. Results revealed that the unfrozen water content had the most significant influence on the model's predictions, followed by displacement and initial water content. The steel structure had no effect on the predictions of the XGB model. Nevertheless, it should be noted that the SHAP analysis results may differ from the actual mechanism because this analysis depends only on the training database.

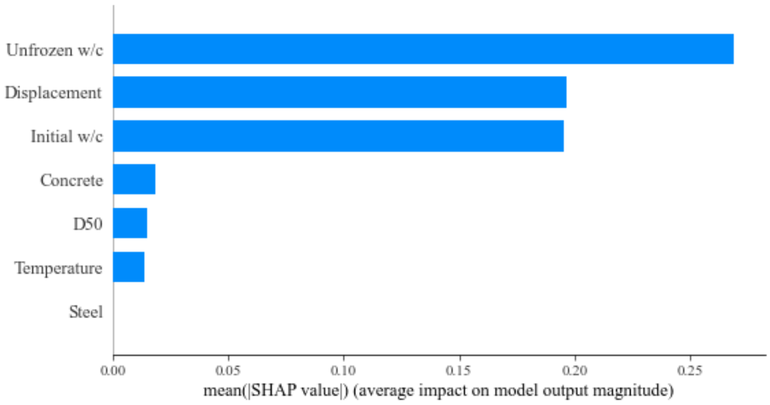


Fig. 3 SHAP analysis result

Finally, the developed XGB model's interpolation and extrapolation capabilities were evaluated under untrained input conditions. Adfreezing stress-displacement curves were generated for various hypothetical conditions, and the adfreezing strength was determined as the maximum adfreezing stress value obtained from each curve. Fig. 4 compares the observed and predicted adfreezing strengths based on the freezing temperature under steel structure conditions. The XGB model provided reasonable predictions within a specific temperature range of -5 to -15°C, demonstrating its capability for interpolation. However, between -15 and -20 degrees, interpolation through this model appeared to be challenging. In addition, the XGB model yielded irrational adfreezing strength predictions beyond the range of the training data (i.e., temperatures above –5°C and below –25°C), highlighting the limitations of extrapolation.

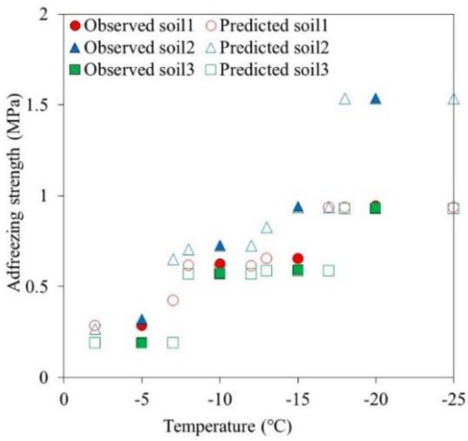


Fig. 4 Adfreezing strength based on freezing temperatures under steel structure conditions

5. CONCLUSIONS

In this study, four machine learning algorithms were utilized to predict the adfreezing behavior under various experimental conditions obtained from the punch shear test. The ensemble models (RF and XGB) with complex structures demonstrated higher accuracy in predicting adfreezing stress compared to the single models (SVR and FNN). The XGB model resulted in the best prediction accuracy. Moreover, the reliability of the XGB model was verified by quantifying prediction uncertainty using a prediction interval, and the influences of input features on the prediction were analyzed through the SHAP value analysis. Finally, the XGB model provided reasonable predictions within the trained data range, but it yielded irrational values outside this range, highlighting the limitations of the data-based approach.

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