Study on Predictive Models for Leaching Behavior of Waste Glasses Based on Machine Learning Algorithms

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1. Introduction

Radioactive waste produced from spent nuclear fuel reprocessing or operation of nuclear power plants has been converted to borosilicate glasses. These glasses are destined to be disposed of in repositories over ten thousands of years. The leaching behavior of waste glasses is essential to reasonably predict the long-term stability of the glasses. In this regard, many studies have been performed to produce data related to glass leaching behavior. Empirical data is made by experiments that simulate the repository environments. Theoretical works has revealed the various mechanisms of glass dissolution. Computational studies are also contributing to the understanding of glass alteration behavior. However, the current phase of glass leaching research is still far from the level of the prediction of glass leaching characteristics for sufficiently long time. In this study, efforts are focused on the examination of predictive models of glass leaching behavior based on machine learning algorithms.

2. Methods

2.1 Input data manipulation

Modeling by machine learning requires many data to find a reasonable model for prediction. Herein, data on glass properties and leaching rates were obtained from a published report [1]. The leaching rates were produced by Product Consistency Test (PCT) and data on B, Li, Na, Si were provided. Feature (sometimes called parameter) selection was followed. Glass leaching could be affected by several factors such as glass composition, melting temperature, cooling method, and testing environment. All glasses were described to be melted at 1150 °C and quickly cooled glasses were only considered. In addition, PCT data obtained by a test at 90 °C were used. Therefore, it is considered that glass composition is the only substantial feature to affect the leaching rates in this research. Among 61 components presented in the report, ones with higher than 0.5 wt% and ones that are told to be related to the leaching property were selected and 42 components were finally chosen as features. As a result, total 1207 PCT data were used as training, cross-validation, and testing dataset. The purpose of this study is to develop a basic predictive model that classifies the durability of glasses based on leaching rates. Therefore, data were labeled to indicate the durability level: 1, 2, and 3 means poor, normal, and good durability.

2.2 Machine learning modeling

Support vector machine (SVM) algorithm, a representative classification algorithm, was used to develop a model. Source codes necessary for the model were obtained from the famous libraries of scikit-learn [2]. As a first step, parameter optimization was performed by adjusting kernel parameters (C, γ) with cross-validation. Then, the model with the optimized parameters was trained by training dataset. Finally, the predictive accuracy was performed by using test dataset.

3. Results and discussion

Fig. 1 shows the result of grid search to find the optimal parameter combination. Gamma and C factors were varied from 0.001 to 100 and the mean scores of 5-fold cross-validation were written in each box. As seen in the heat map, most scores remain 0.75 even after parameter adjustment. The best score is shown in the brightest box which corresponds to (C, γ)=(10, 100). This score means that the prediction accuracy is 87% after parameter optimization.

The accuracy score is not enough to validate model performance. Error matrix was calculated to see how precise the model predicts for each label. As indicated in Fig. 2, the number of precise prediction for the label 1, 2, and 3 is 25, 149, 7, respectively. The accuracy score for the label 1, 2, and 3 is 0.81, 0.89, and 0.88, respectively. This result indicates that the classification into low durable glass group by using the current model is relatively inaccurate. Further research should be performed to modify the performance of the model. Machine learning based models are thought to suggest the optimized glass compositions that improve the stability of the glass.

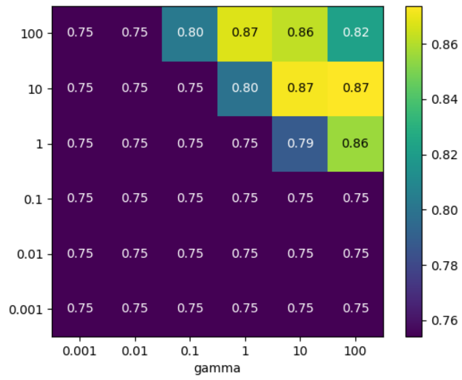

Fig. 1. Result of grid search for parameter optimization.

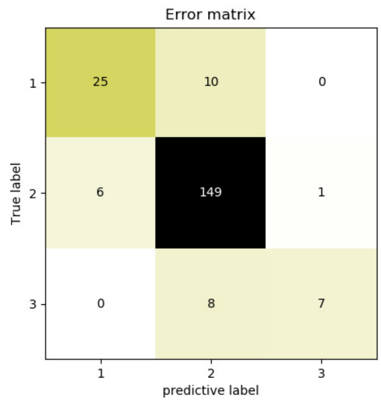

Fig. 2. Error matrix of the predictive model.

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[1] J. Vienna, D. Kim, P. Hrma. “Database and Interim Glass Property Models for Hanford HLW and LAW Glasses”, PNNL-14060, Pacific Northwest National Laboratory, (2002).

[2] http://scikit-learn.org/stable/