Comparison of regression and classification Machine Learning algorithms for determining excavation damage zones depths

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ABSTRACT: During the construction of underground excavations, the development of excavation damage zones (EDZs) is a crucial factor in designing permeability-sensitive excavations, such as deep geological repositories for nuclear waste. In this study, regression and classification machine learning (ML) models were employed. Specifically, k-nearest neighbors (KNN) and multi-layer perceptron (MLP) were used for both models. The aim of the regression ML models was to predict the depth of damage based on the maximum tangential stress around the opening and the crack initiation (CI) threshold. In contrast, the classification ML models aimed to determine different EDZ zones using the same features. After comparing the ML models with each other and with the traditional regression approach, it was concluded that MLP outperforms KNN for both models. Moreover, MLP exhibits consistency with the traditional regression lines. Thus, MLP can be effectively utilized for regression in higher-dimension modeling with a greater number of features.

Keywords: Excavation Damage Zones, Machine Learning, Regression, Classification, K-Nearest Neighbor, Multi-Layer Perceptron.

1 INTRODUCTION

Excavation of an underground opening results in changes in the geomechanical properties of the rock surrounding the opening. During the construction process, excavation-induced cracks are initiated and expand into the rock once the stress concentration exceeds the rock's failure strength. This continues until a new stress equilibrium condition is reached. Excavation Damage Zones (EDZs) have been studied for a long time (Kelsall et al. 1984). It is crucial to have a good understanding of the degree and extent of the EDZs for designing deep geological repositories for nuclear waste (Olsson & Winberg 1996), since the new cracks change the permeability of the rock.

Empirical methods are used in a variety of ways, for example, to estimate rock mass strength and to establish rock mass classes based on RMR or GSI. Machine Learning (ML) algorithms are well suited to learning underlying patterns in large data sets. For example, a convolutional neural network study for predicting tunnel liner yield demonstrates the benefit of ML (Morgenroth et al. 2022). ML algorithms are beginning to be leveraged for subsurface applications opening research opportunities.

2 EXCAVATION DAMAGE ZONES (EDZS)

Understanding the depth of damage around an excavation is crucial for the design of any type of underground space, as it can be associated with the stability of the structure. Moreover, in the case of deep geological repositories, where the damage zone can increase permeability and form a potential flow pathway for contaminants, it is critical to determine the depth of damage. The continuous connectivity of the EDZ parallel to the excavation axis could lead to a breach of the geological barrier should radionuclides breach any of the various engineered barriers present in a repository (Perras & Diederichs 2016). As shown in Figure 1 the excavation damage zones can be divided into five regions. The damage that is induced during construction due to blasting or other construction tools form the construction damage zone (CDZ). The region where damage is observed as interconnected macro-fractures is known as the highly damage zone (HDZ). The region with connected micro-damage and significant dilation is referred to the inner excavation damage zone (EDZ_i) and the region with partially connected to isolated micro-damage that has no significant dilation is called the outer excavation damage zone (EDZ_o). Beyond the EDZ_o region is the excavation influence zone (EIZ), where only elastic changes occur (Perras & Diederichs 2016).

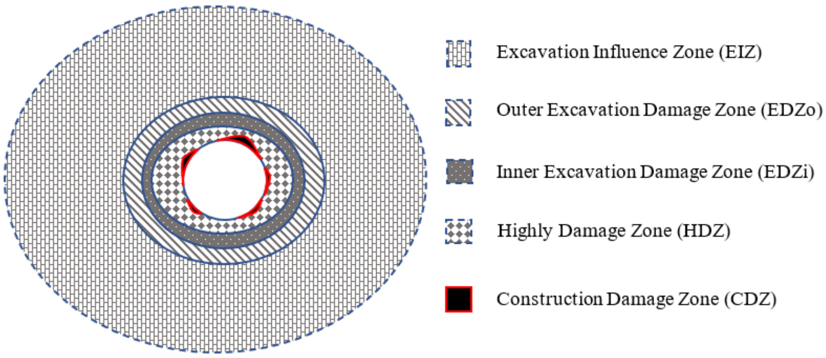

Figure 1. Schematic representation of the EDZs around an underground opening.

In-situ measurement of the EDZs from a variety of case studies compiled by Perras & Diederichs (2016) are presented in Figure 2, where the maximum tangential stress is normalized by the crack initiation (CI) threshold and plotted against the depth of damage that is normalized by the radius of the tunnel. Martin et al. (1999) originally introduced a linear empirical depth of failure criteria then Diederichs (2007) expanded the empirical dataset and demonstrated mechanistically that a linear depth of failure was best predicted when normalizing by CI rather than UCS. Perras & Diederichs (2016) discussed how these linear depth of failure equations mostly divided the EDZ_i from EDZ_o. As shown in Figure 2, there is a divergence from the linear empirical depth of failure by Diederichs' (2007) as the σ_{max}/CI and the depth of failure increases. However, a numerically focused depth of failure analysis indicated that a non-linear fit may be more suitable for predicting the depth of EDZs (Perras & Diederichs 2016) at higher stress levels than the empirical data. The numerical analysis utilized the damage initiation and spalling limit (DISL) approach developed by Diederichs (2007), to represent brittle spalling behavior and to define the limiting stress envelops (peak and residual) using the generalized Hoek-Brown formula. The non-linear curves in Figure 2 are traditional regression models of the numerical data that were plotted using the stats-model library and they aligned with the empirical EDZs data. As the goal is to enhance the accuracy of regression models, the gap rises between traditional regression approaches and the imperative to leverage the potential of ML algorithms. By employing advanced ML algorithms to effectively handle non-linearity and high dimensional data, the limitation of conventional regression methods can be overcome.

3 MACHINE LEARNING

Machine learning is a technique that computers learn from experience, by examining data and improving the algorithms' performance for prediction (Liu 2021). The main task when using machine learning is to develop learning algorithms that use data to build a model and then use the model to make prediction on the unseen data (Liu 2021). Machine learning models fall into four primary categories, supervised learning, unsupervised learning, semi-supervised learning, and reinforcement learning. The difference is about the data that is fed to the learning algorithm (Géron 2019). Two sub-categories of supervised learning are regression and classification. In classification the algorithm must learn how to classify data into separate groups, whereas in regression it has to learn how to predict a target numeric value (Géron 2019).

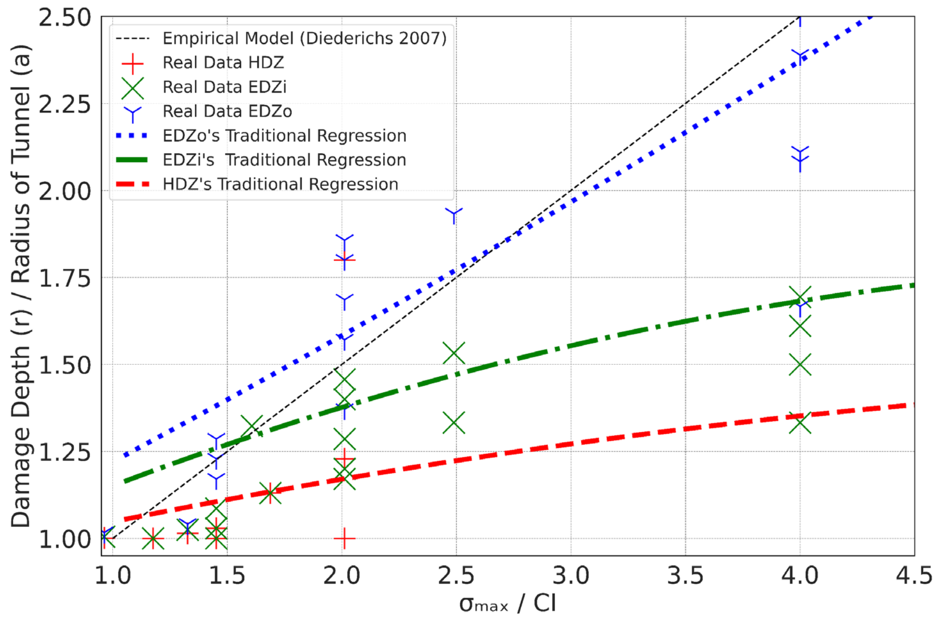

Figure 2. Comparison of in-situ depth of EDZs with traditional regression curves of the original numerical data from Perras & Diederichs (2016) and the empirical depth of failure line from Diederichs (2007).

3.1 *Algorithms for Regression and Classification ML models*

Two different algorithms were used in this study; k-nearest neighbor (KNN) and multi-layer perceptron (MLP). KNN is one of the fundamental classification schemes that is also used for regression. In order to make a prediction for unseen data, the algorithm uses Euclidean distance, equation (1), to measure the distance to find the closest neighbors (Muller & Guido 2020).

$$distance = \sqrt{(X_2 - X_1)^2 - (Y_2 - Y_1)^2} \tag{1}$$

Where (X_1, Y_1) and (X_2, Y_2) are the coordinates of two points. KNN is also used for regression in a sense that a target value of an unknown data can be predicted based on the KNN target values (Muller & Guido 2020). An MLP is comprised of an input layer, hidden layers, and an output layer. Each hidden layer has different connection weights that are initialized randomly. An MLP uses backpropagation to first make a prediction that measures the error and then goes back to the layer to compute the error contribution for each connection, subsequently adjusting the connection weights to minimize the error (Géron 2019).

3.2 *Application of ML to EDZ depth prediction*

Regression ML models help to predict the damage depth as a continuous quantity by using the maximum tangential stress around the opening, and the crack initiation (CI) threshold. Whereas the classification ML models determine which EDZ zone the damage depth belongs to. The code was written in Python 3.11.1 and the scikit-learn ML package was used. The data that fed into the ML models are from the numerical study of Perras & Diederichs (2016). For the regression ML model, the model was trained using 80% of the data (i.e., the training set). The hyperparameters were tunned to give the best results then the calibrated model was tested on the remaining 20% of data (i.e., test set). The same procedure applied for the classification ML models, however, the stratified k-fold methods was used for hyper parameter tunning for the training set.

4 RESULTS

4.1 Regression Models

For each EDZs (HDZ, EDZ_i, and EDZ_o), ML regression models were developed and compared with each other and the traditional regression model (the base model). Various evaluation metrics were utilized to assess the performance of the regression models, including R^2, mean absolute error (MAE). The R^2 value ranges from 0 to 1, where a value of 1 indicates that the ML algorithm accurately predicts the dependent variable using the independent variable(s). The general procedure for both ML models involved calibrating the algorithm using the training set and then inputting the independent variable, σ_{max}/CI, to the model in order to predict the dependent variable, Damage Depth/Radius of tunnel. In Figure 3, the regression lines were plotted based on the predicted values of damage depth/radius of the tunnel.

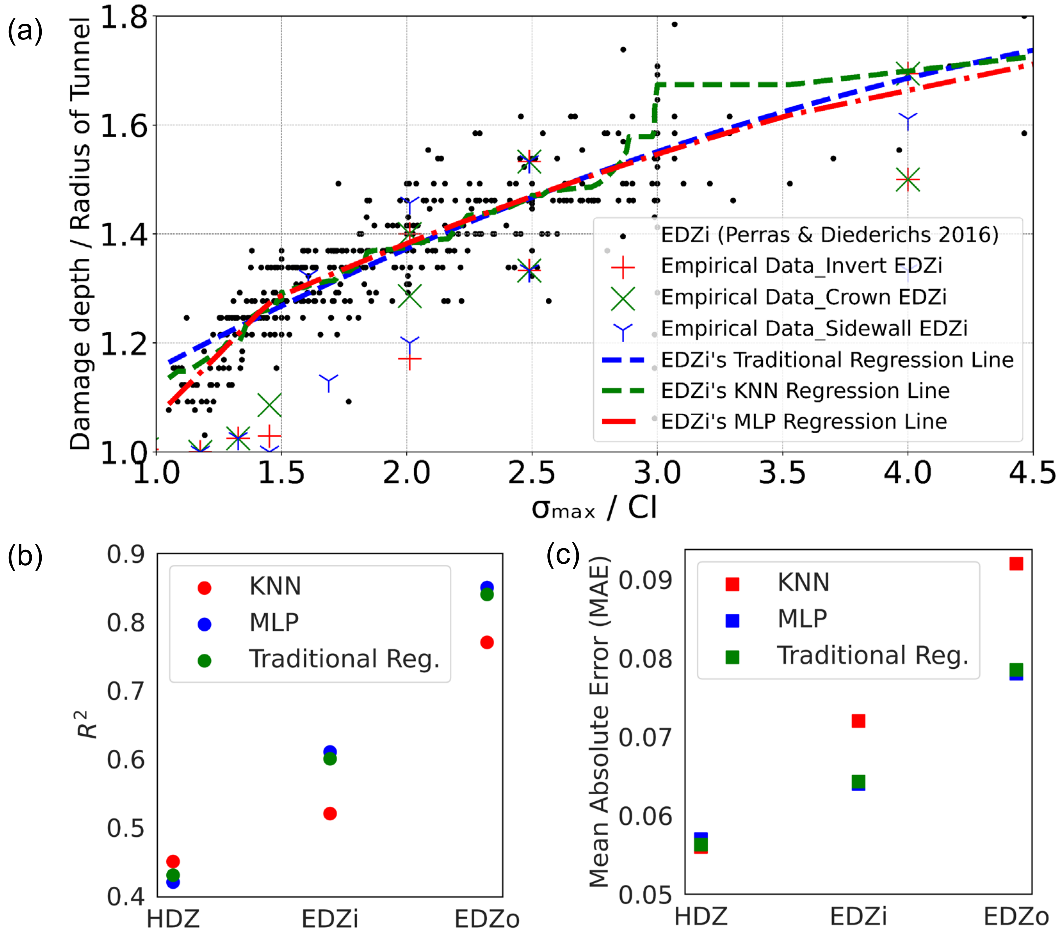

Figure 3. (a) Traditional regression, KNN and MLP ML regressions for EDZ_i, (b) R^2 values for KNN and MLP regression models, (c) MAE for KNN and MLP regression models.

Figure 3-a illustrates an example of the regression ML models for EDZ$_i$. It shows the strong consistency between the MLP ML regression line and the traditional regression model. Notably, the MLP model demonstrates superior generalization when σ_{max}/CI is less than 1.5. Comparing the R^2 and MAE values across different EDZs for both ML models (Figure 3-b and Figure 3-c), it becomes evident that the MLP outperforms the KNN model. MLP exhibits lower MAE for EDZ$_i$ and EDZ$_o$, and comparable values for HDZ. Additionally, MLP achieves higher R^2 values for EDZ$_i$. In conclusion, MLP proves to be more effective than KNN for regression tasks.

4.2 Classification Models

The performance of classification models was evaluated using several key metrics, including the confusion matrix, receiver operating characteristic (ROC) curve, and area under the ROC curve (AUC). The confusion matrix provides a summary of a classification model's performance. It is presented as a table, where the diagonal elements represent the number of correctly classified instances for each class. The ROC curve is a graphical representation of the performance of a binary classification model. A superior classifier will have a curve that is closer to the top-left corner of the plot, indicating higher accuracy of the model. By considering these metrics, researchers can make informed decisions about the efficacy of each model.

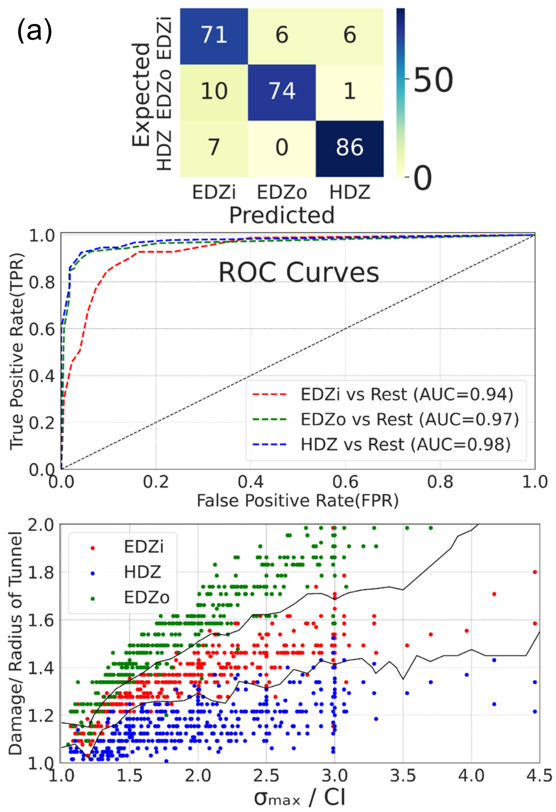

Figure 4. The evaluation metrics for classification ML models; column (a) for KNN and column (b) for MLP. From top to bottom: Confusion Matrix, ROC Curves, Decision Boundaries.

Figure 4 presents a comprehensive comparison of the KNN and MLP classifications metrics. In general, the ROC curve is conducted for binary classification, therefore each EDZ was binarized against the remaining EDZs. Thus, three ROC curves were plotted, for both ML models. Although a comparison of the evaluation metrics suggests similar or slightly better performance for the MLP model, it is when the decision boundaries are examined that the superiority of the MLP approach as a classifier becomes apparent. The MLP model exhibits a noise-free decision boundary that does not show overfitting, unlike the KNN. Additionally, the MLP performs better when σ_{max}/CI is less than

1.5, effectively classifying the EDZs. So, it can also be concluded that the MLP model outperforms the KNN model in classification tasks.

5 CONCLUSION

Understanding the impact of creating an excavation on the surrounding rocks and the stability of underground structures is crucial. Fractures and damage resulting from excavation can significantly affect subsurface stability and permeability within the HDZ and EDZ_i. Therefore, accurate prediction of the depth of damage is critical for permeability sensitive underground structures. Empirical methods introduced by Martin et al. (1999) and Diederichs (2007) have successfully predicted the depth of brittle failure, however, Perras & Diederichs (2016) demonstrated the accuracy of nonlinear prediction curves to predict the depth of EDZs. This research follows a similar path by applying machine learning (ML) algorithms on the existing numerical data. Two ML regression algorithms, K-Nearest Neighbors (KNN) and Multi-Layer Perceptron (MLP) were employed to demonstrate that ML approaches can make similar, if not better, predictions than the traditional regression method. The regression ML models aimed to predict damage depth based on the maximum tangential stress around the opening and the crack initiation (CI) threshold. Subsequently, KNN and MLP were employed for classification purposes that aimed to determine different excavation damage zone (EDZ) regions using the same features. For regression, MLP outperformed KNN, showing consistency with the traditional regression model and an advantage when σ_{max}/CI was less than 1.5. For classification, MLP exhibited superior performance by avoiding overfitting in decision boundaries compared to the KNN model. Thus, it can be concluded that the MLP outperforms the KNN approach in this study. This research serves as a preliminary study to validate the performance of ML models compared to traditional regression approach. With this goal achieved, the next stage would involve modeling more complex regression models using additional numerical inputs as ML features to predict the depth of EDZs and then perform input variable selection to figure out which input parameter has more influence on damage depth.

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