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Estimation of the TBM advance rate under hard rock conditions using XGBoost and Bayesian optimization

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Abstract

The advance rate (AR) of a tunnel boring machine (TBM) under hard rock conditions is a key parameter in the successful implementation of tunneling engineering. In this study, we improved the accuracy of prediction models by employing a hybrid model of extreme gradient boosting (XGBoost) with Bayesian optimization (BO) to model the TBM AR. To develop the proposed models, 1286 sets of data were collected from the Peng Selangor Raw Water Transfer tunnel project in Malaysia. The database consists of rock mass and intact rock features, including rock mass rating, rock quality designation, weathered zone, uniaxial compressive strength, and Brazilian tensile strength. Machine specifications, including revolution per minute and thrust force, were considered to predict the TBM AR. The accuracies of the predictive models were examined using the root mean squares error (RMSE) and the coefficient of determination (R^2) between the observed and predicted yield by employing a five-fold cross-validation procedure. Results showed that the BO algorithm can capture better hyper-parameters for the XGBoost prediction model than can the default XGBoost model. The robustness and generalization of the BO-XGBoost model yielded prominent results with RMSE and R^2 values of 0.0967 and 0.9806 (for the testing phase), respectively. The results demonstrated the merits of the proposed BO-XGBoost model. In addition, variable importance through mutual information tests was applied to interpret the XGBoost model and demonstrated that machine parameters have the greatest impact as compared to rock mass and material properties.

Keywords: TBM performance; Advance rate; XGBoost; Bayesian optimization; Predictive modeling

1 Introduction

Predicting tunnel boring machine (TBM) performance is critical for estimating the project costs and duration of mechanized tunneling projects. The prediction of TBM performance depends on the accurate estimation of the advance rate (AR), penetration rate (PR), and/or utilization coefficients (AR/PR) (Sapigni, Berti, Bethaz, Busillo, & Cardone, 2002; Yagiz, Gokceoglu, Sezer, & Iplikci, 2009; Xu, Zhou, Asteris, Jahed Armaghani, & Tahir, 2019; Gao, Wang, et al., 2020, Gao, Amar, et al., 2020; Zhou, Bejarbaneh, et al. 2020). In particular, AR is the actual distance mined or supported divided by the total time of the operations and includes downtimes for TBM

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maintenance, tunnel failure, machine breakdown, etc. Over the years, numerous TBM performance prediction models have been developed using empirical, theoretical, and semi-empirical approaches (Graham, 1976; Barton, 1999; Sapigni et al., 2002; Yagiz, 2008; Gong & Zhao, 2009; Hamidi, Shahriar, Rezai, & Rostami, 2010; Zhang & Goh, 2013; Goh, Zhang, Zhang, Xiao, & Xiang, 2018; Armaghani, Mohamad, Narayanasamy, Narita, & Yagiz, 2017, 2018; Koopialipoor, Nikouei, et al., 2019, Koopialipoor, Tootoonchi, et al., 2019, 2020; Zhang, Li, Wu, Li, Liu, et al., 2020; Zhang, Li, Wu, Li, Goh, et al., 2020; Zhou, Bejarbaneh, et al., 2020). However, because these empirical and theoretical investigations focus on only a few important parameters, their performance predictions are unacceptable, and most of them are applicable only to their specific projects (Armaghani, Koopialipoor, Marto, & Yagiz, 2019).

In addition to empirical and theoretical investigations, many researchers have applied various artificial intelligence (AI) techniques for TBM performance prediction. For example, Grima, Bruines, and Verhoef (2000) proposed the neuro-fuzzy method to model the performance of TBMs for 640 TBM projects. Zhao, Gong, Zhang, and Zhao (2007) applied a TBM performance prediction model using ensemble neural networks with 47 sets of data. In another investigation, Yagiz and Karahan (2011) implemented a particle swarm optimization (PSO) technique for forecasting the TBM PR in hard rock. Recently, Armaghani et al. (2019) developed two hybrid optimization techniques based on PSO and an imperialist competitive algorithm (ICA) for predicting the AR of TBM in different weathered zones of granite. The aforementioned models have both advantages and disadvantages, and efforts have been made to enhance the accuracy of these models and to minimize their shortcomings. Understanding and predicting the performance of TBM still poses a considerable challenge for TBM excavation under hard rock conditions.

Extreme gradient boosting (XGBoost) proposed by Chen and Guestrin (2016) is a powerful ensemble learning algorithm based on a gradient boosting system (Friedman, 2001; Xia, Liu, Li, & Liu, 2017; Zhou et al. 2015, 2016, 2018). More specifically, XGBoost is a powerful data-mining tool that has been widely used and proven effective in many regression and classification problems (Le, Nguyen, Zhou, Dou, & Moayedi, 2019; Zhou, Li, Wang, et al., 2019; Zhou, Li, Yang, et al., 2019; Ding, Nguyen, Bui, Zhou, & Moayedi, 2020; Wang et al., 2020; Zhang et al., 2019, Zhang, Wu, et al., 2020; Zhang, Zhang, Wu, Goh, & Wang, 2020). Accordingly, we decided to illustrate the capability of the XGBoost technique in TBM AR prediction. In addition, tuning the hyper-parameters of XGBoost models for TBM datasets is also worthwhile. Thus, the Bayesian optimization (BO) algorithm is used to optimize the hyper-parameters of XGBoost. This is an innovative work, as TBM AR prediction under hard rock conditions has not been previously investigated in the manner described in this study. In the following sections, following descriptions of the data and case study, AI models and their modeling process are explained. The results of the AI models in predicting the TBM AR are then assessed and discussed. Finally, a sensitivity analysis of our data is conducted to identify the most important parameters for the TBM AR.

2 Materials and methods

2.1 Dataset preparation

In this study, 1286 datasets from the Peng Selangor Raw Water Transfer (PSRWT) tunnel project in Malaysia were prepared for use as a comprehensive database to predict the AR of TBM and in the construction of artificial intelligence models based on XGBoost. This database consists of 560, 553, and 173 datasets of fresh zone of rock mass, slightly weathered zone of rock mass, and moderately weathered zone of rock mass, respectively. In each section of the tunnel, relevant machine factors, rock material, and mass characteristics were recorded, including rock mass strength properties, joint condition, revolution per minute (RPM), weathering zone (WZ), uniaxial compressive strength (UCS), rock mass rating (RMR), Brazilian tensile strength (BTS), rock quality designation (RQD), and trust force per cutter (TFC).

The established research database contains total eight variables (i.e., seven input characteristics affecting the TBM AR and TBM AR as model output), where the input variables can be divided into rock mass properties (RMR, WZ, and RQD), rock material properties (UCS and BTS), and machine characteristics (TFC and RPM). In the modeling process, to facilitate the use of WZ data, a rating system for each WZ was adopted. As noted by the International Society for Rock Mechanics (1981), a typical rock weathering profile is composed of six weathering grades: fresh, slightly weathered, moderately weathered, highly weathered, completely weathered, and residual soil (see Table 1). This classification is mainly based on the discoloration and decomposition of the rock material. After tunnel mapping from 34 740 m of PSRWT tunnel excavated by TBMs, the following was investigated: a total of 12 649 m consisting of 5443 m in fresh, 5530 m in slightly weathered, and 1676 m in moderately weathered zones. The ratings for the fresh, slightly, and moderately weathered zones were 1, 2, and 3, respectively. It should be noted that a similar procedure was conducted in the work of Benardos and Kaliampakos (2004).

The range and mean values of the influencing factors (BTS, UCS, RMR, RQD, WZ, TFC, and RPM) together with the AR of the TBM are listed in Table 1. It can then be seen from the matrix analysis chart presented as Fig. 1 that a correlation existed between the input variables in the database and between the input parameters and output of AR. In Fig. 2, the violin plot depicts the distribution of each input and output and provides an analysis of outliers.

Table 1
Description of variable definitions, ranges, and categories.

Category	Symbol	Unit	Parameter description (min–max)	Mean	Note
Input	BTS	MPa	(4.69–15.68)	10.321	Rock material properties
Input	UCS	MPa	(40–194)	135.128	Rock material properties
Input	RMR	–	(44–95)	72.894	Rock mass properties
Input	RQD	Percentage	(6.25–95.00)	54.259	Rock mass properties
Input	WZ	–	(1–3)	1.699	Rock mass properties
Input	TFC	kN	(80.60–565.84)	301.514	Machine characteristics
Input	RPM	$r{\cdot}min^{-1}$	(4.04–11.95)	8.827	Machine characteristics
Output	AR	$m{\cdot}h^{-1}$	(0.017–5)	1.083	

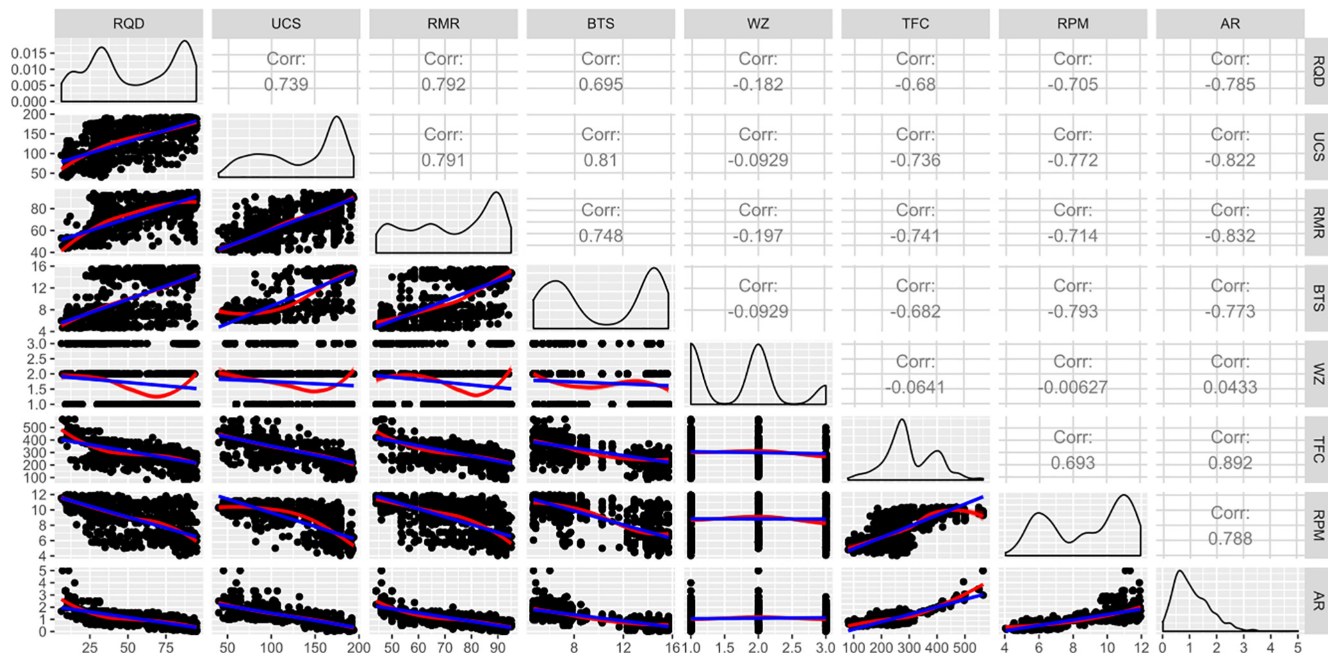

Fig. 1. Scatterplot matrix of TBM dataset with correlation.

2.2 Extreme gradient boosting (XGBoost)

XGBoost, proposed by Chen and Guestrin (2016), is a scalable machine learning system associated with tree boosting. This system has been applied to many engineering fields and has produced excellent performance due to the advantages of effective tree pruning, regularization, and parallel processing.

As the archetype of XGBoost, gradient boosting combines the predictions of a few “weak” learners into a “strong” learner in an iterative manner (Le et al., 2019; Ding et al., 2020; Zhang, Li, Wu, Li, Goh, et al., 2020, Zhang, Wu, et al., 2020). XGBoost utilizes the residual to calibrate the previous predictor at each iteration; this is a process of optimizing the loss function. In addition, to reduce the risk of overfitting in the calibration process, XGBoost adds regularization into the objective function, which can be described by

$$J(\Theta) = L(\Theta) + \Omega(\Theta) \tag{1}$$

where Θ is the parameter trained from the given data; Ω denotes regularization, which is meant to avoid overfitting because it can control the complexity of the model; L indicates the training loss functions (i.e., square/logistic loss), which measures how well the model fits the training data. Equation (2) is a prediction function; according to the theory of decision tree (DT), the output of the model $\hat{y}_i$ depends on voting or the average of a collection F of k trees:

$$\hat{y}_i = \sum\nolimits_{i=1}^{k} f_k(x_i), \quad f_k \in F. \tag{2}$$

The objective function at the t time iteration can be described by a more specific mathematical model given by

$$J^{(t)} = \sum\nolimits_{i=1}^{n} L(y_i, \hat{y}_i) + \sum\nolimits_{k=1}^{t} \Omega(f_k). \tag{3}$$

Here, n is the number of predictions, and $\hat{y}^{(t)}{}_i$ can be defined as

$$\hat{y}^{(t)}{}_i = \sum\nolimits_{k=1}^{t} f_k(x_i) = \hat{y}_i{}^{(t-1)} + f_t(x_i). \tag{4}$$

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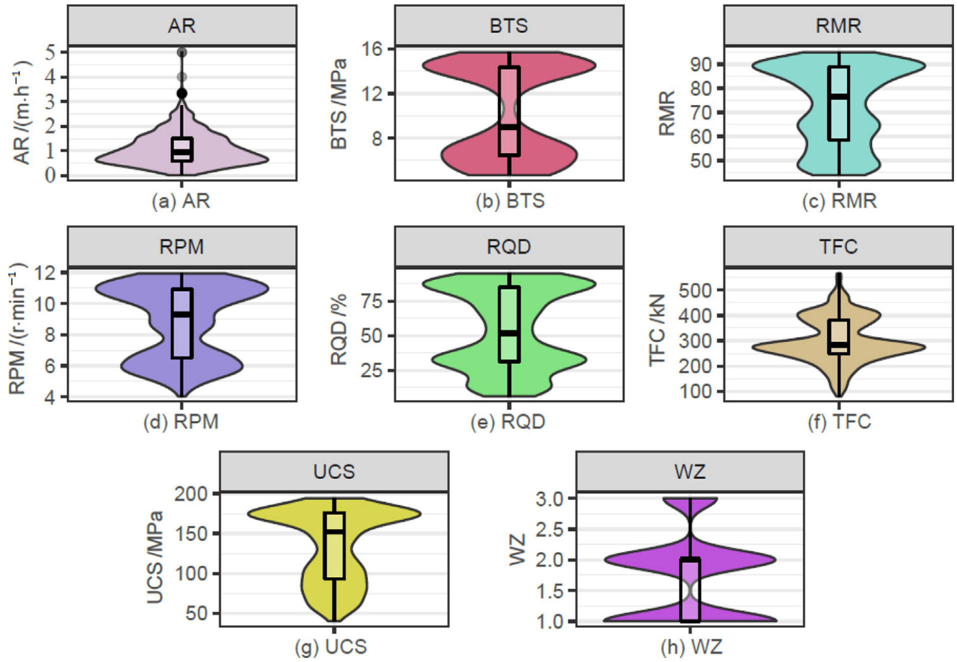


Fig. 2. Violin plots of TBM database used in the XGBoost modeling process.

As illustrated by Chen and Guestrin (2016), the regularization term $\Omega(f_k)$ for the DT is denoted as

$$\Omega(f_k) = \gamma T + 0.5\lambda \sum_{j=1}^{T} {\omega_j}^2, \tag{5}$$

where λ scales the penalty, T represents the number of leaves in the DT, in which the complexity of each leaf is indicated by γ, and ω is the vector of scores on the leaves. Then, second-order (instead of first-order) Taylor expansion in general gradient boosting is applied to the loss function (LOF) in XGBoost (Chen & Guestrin, 2016; Xia et al., 2017). When the mean square error (MSE) is assumed as the LOF, the objective function can be obtained by the following equation:

$$J^{(t)} \approx \sum_{i=1}^{n} \left[g_i \omega_{q(x_i)} + \frac{1}{2}\left(h_i \omega_{q(x_i)}^2 \right) \right] + \gamma T + \frac{1}{2}\lambda \sum_{j=1}^{T} {\omega_j}^2, \tag{6}$$

where g_i and h_i represent the first and second derivatives of the MSE loss function, respectively, and q is a function that assigns a data point to the corresponding leaf.

Obviously, the LOF in Eq. (6) is subject to the sum of the loss values for each data sample. Because each data sample only corresponds to one leaf node, the sum of the loss values of each leaf node can also be used to describe the LOF, namely,

$$J^{(t)} \approx \gamma T + \sum_{j=1}^{T} \left[\left(\sum_{i \in i_j} g_i \right) \omega_j + 0.5 \left(\sum_{i \in i_j} h_i + \lambda \right) \omega_j^2 \right]. \tag{7}$$

Accordingly, G_j and H_j are defined as

$$G_j = \sum_{i \in i_j} g_i, H_j = \sum_{i \in i_j} h_i, \tag{8}$$

where I_j indicates all the data samples in leaf node j.

Overall, the optimization of the objective function can be converted to a process of finding the minimum of a quadratic function. In other words, after a certain node in the DT is split, the objective function is used to evaluate the change in model performance. If the model performance is greater than previously, this split will be adopted; otherwise, the split will be stopped. In addition, regularization is helpful to avoid over-fitting.

2.3 BO

Many optimizations assume that the objective function $f(x)$ is a known mathematical form and a convex function that is easy to evaluate. For parameter tuning, the objective function is unknown and is a computationally expensive non-convex function. Therefore, the commonly used optimization methods have difficulties in playing a critical role, and the BO method is extremely powerful when the objective function is unknown and the calculation complexity is high. BO uses prior knowledge to approach the posterior distribution of the unknown objective function and then selects the next sampled hyperparameter combination according to the distribution.

In general, selecting hyperparameters for optimal performance is desirable. Therefore, hyperparameter selection can be regarded as an optimization problem, that is, a performance function $f(x)$ whose optimal hyperparameter value is an independent variable. BO has been proven to be superior to other global optimization algorithms on many challenging optimization benchmark functions (Jones, 2001). To use the BO technique, we need an efficient means of modeling the distribution of the objective function. If x contains continuous hyperparameters, there will be an infinite number of x to model $f(x)$ (i.e., to construct a distribution for the objective function). For this problem, the Gaussian process (Williams, 1998; Rasmussen 2004; Rasmussen and Williams 2005) generates a multidimensional Gaussian distribution, which is a high-dimensional normal distribution sufficiently flexible to model any objective function. In other words, BO assumes that the function to be optimized is $f: \boldsymbol{X} \rightarrow \mathbb{R}$, where $\boldsymbol{X} \subset \mathbb{R}^n, n \in N$. Then, in each iteration $(t = 1,2,\cdots,T)$, $f(x_t), x_t \in \boldsymbol{X}$ is obtained according to the acquisition function (α_t). Then, a noisy observation $y_t = f(x_t) + \varepsilon$ is obtained, where ε follows the zero-mean Gaussian distribution $\varepsilon \sim \mathcal{N}(0, \sigma^2)$, and σ is the noise variance. Then, new observations (x_t, y_t) are added to the observation data, and then the next iteration is performed. BO makes the most of the information from the previous sampling point through the learning of the objective function and finds the parameters that improve the result to the global optimum. The algorithm tests the most likely point given by the posterior distribution.

In this study, XGBoost is the baseline model for forecasting the TBM AR, and the BO technique is applied to search the optimal hyperparameters of the XGBoost model. In this regard, the BO algorithm is used to optimize five parameters involved in the performance of the XGBoost model, including Num_boosting_rounds, Max_depth, Learning_rate, Reg_alpha, and Reg_lambda. Notably, the optimal XGBoost model is determined by the minimum value of the root mean square error (RMSE). Figure 3 displays the analytical process of the BO-XGBoost model in estimating the TBM AR from the beginning to the end.

2.4 Verification and evaluation of the XGBoost-based model

In this study, a training set was employed to build the predictive model, and a test set was used to examine the trained model. In addition, with the aim of evaluating the reliability of the hybrid BO-XGBoost model effectively, the relevant evaluation indicators, namely, the coefficient of determination (R^2) and RMSE, were applied to interpret the relationship between the predicted and observed values. RMSE represents the standard deviation of the fitted error between the predicted and observed values. The value of R^2 represents the percentage of the square of the correlation between the predicted and actual values of the target variable. The calculation formulas of the evaluation indicators are presented as follows (Li et al., 2020; Shi, Zhou, Wu, Huang, & Wei, 2012; Gao, Wang, et al., 2020, Gao, Amar, et al., 2020; Guo, Zhou, Koopialipoor, Armaghani, & Tahir, 2019; Bui et al., 2020; Yong et al., 2020; Yu et al., 2019; Yu, Shi, Zhou, Chen, & Qiu, 2020; Yu, Shi, Zhou, Chen, Miao, et al., 2020; Zhang, Li, Wu, Li, Liu, et al., 2020; Zhang, Li, Wu, Li, Goh, et al., 2020; Zhang, Wu, Zhong, Li, & Wang, 2020; Zhou, Li, & Shi, 2012, 2017; Zhou, Li, Arslan, Hasanipanah, & Amnieh, 2019; Zhou, Li, Wei, et al., 2019; Zhou, Guo, et al., 2020; Zhou, Li, et al., 2020):

$$\mathrm{RMSE} = \sqrt{\sum\nolimits_{i=1}^{N} (\widehat{y}_i - y_i)^2 / N}, \tag{9}$$

$$R^2 = 1 - \frac{\sum_i (y_i - \widehat{y}_i)^2}{\sum_i (y_i - \bar{y}_i)^2}, \tag{10}$$

where y_i represents the observed value, $\hat{y}_i$ is the predicted value of the model, $\bar{y}_i$ represents the average of the observed values, and N denotes the number of samples in the training or testing stages.

3 Results and discussion

For the sake of predicting the TBM AR under hard rock conditions, the BO algorithm was combined with XGBoost (i.e., BO-XGBoost). Based on the aforementioned optimization results, a hyperparameter configuration with a higher prediction performance than the default XGBoost model was obtained. Table 2 shows the parameter search space and parameter adjustment selection of the XGBoost model in the BO process during TBM AR prediction. The initial sample of the five pairs of XGBoost hyperparameters (shown in Table 2) were randomly sampled from search space X, the number of iterations in the BO was fixed at 100, and the associated five-fold cross-validation RMSE values were obtained after the XGBoost model was trained. Thus, the optimal hyperparameters of the XGBoost model could be finally determined when the model had the lowest cross-validation RMSE value. In addition, Fig. 4 plots the fitness values of the BO algorithm with the number of iterations in the process of parameter optimization. It can be seen that as the number of iterations increased, the fitness gradually stabilized. Variations in the parameter values during the optimization process are plotted in the dependency plot of Fig. 5, and the optimal parameters that were obtained are marked on it. It can be seen from the partial dependence plot that “Num_boosting_rounds”, “Max_depth”, and “Learning-rate” had the greatest impact on the target optimization.

To better understand the performance of the BO-XGBoost, the measured and predicted AR values of the training and testing datasets are presented in Fig. 6. The figure shows that the AR results predicted by the BO-XGBoost model were closer to their measured values than were those of the default XGBoost predictive model. Based on the optimized hyperparameter results (see Table 3), the prediction accuracy of the BO-XGBoost test set after the hyperparameters were adjusted was higher than that of the default XGBoost model. The R^2 and RMSE values were 0.9806 and 0.0967 for the BO-XGBoost model, respectively, whereas they were 0.9399 and 0.1703 for the XGBoost model, respectively. This proved that, for the TBM dataset that predicts AR, BO-XGBoost could better fit the complex relationship between the factor variables

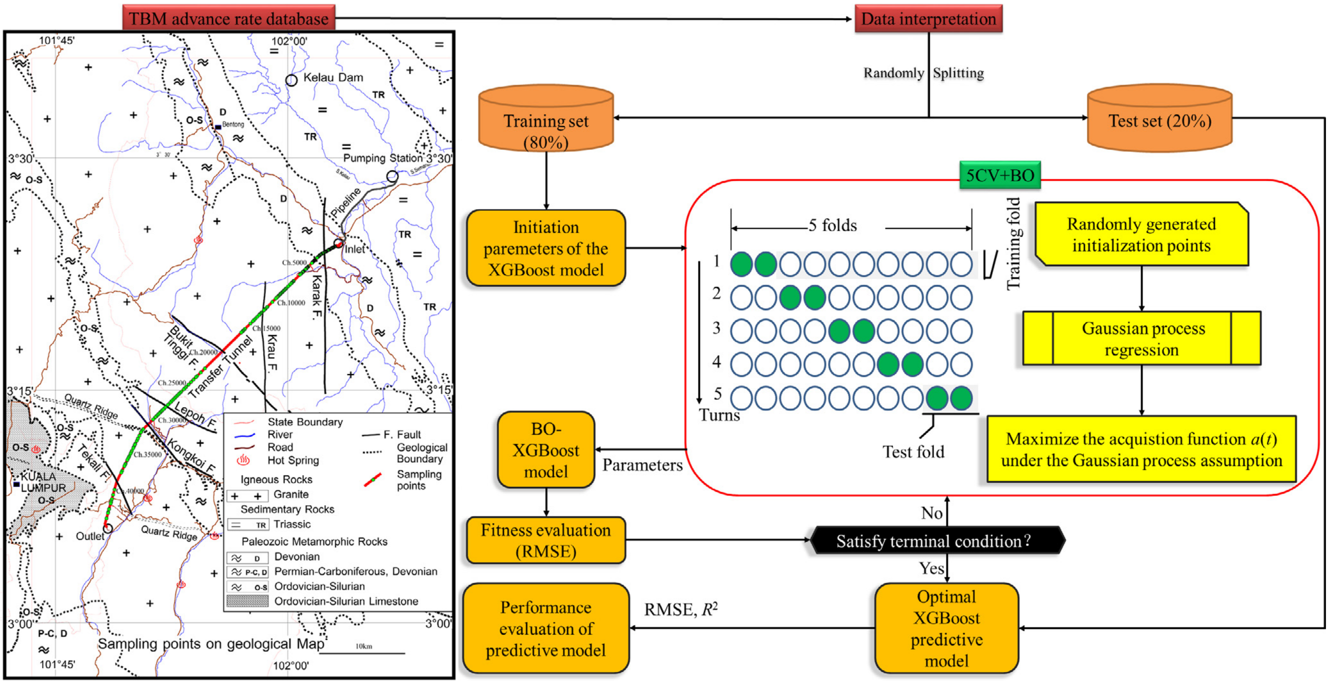


Fig. 3. Overall analytical process of the BO-XGBoost model.

Table 2
Search space and optimal hyperparameters for each of the XGBoost parameters in the BO tuning process.

XGBoost hyperparameters	Lower limit	Upper limit	Optimal values
Num_boosting_rounds	1	150	103
Max_depth	1	15	15
Learning_rate	0.000 01	1	0.152
Reg_alpha	1	15	1
Reg_lambda	1	15	13

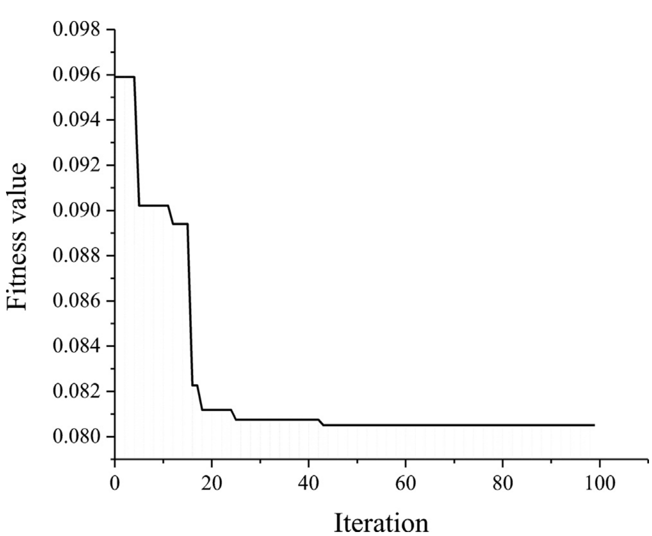


Fig. 4. Fitness and iteration relationship during BO.

affecting AR and TBM and that the generalization ability was better.

Finally, the BO-XGBoost prediction model obtained satisfactory prediction results, showing favorable adaptability. Therefore, it is suitable for evaluating the TBM AR.

Results from previous relevant studies reveal that the BO-XGBoost model developed in this study is superior to the earlier models. For example, Armaghani et al. (2019) concluded that their ICA-artificial neural network (ANN) model with an R^2 of 0.951 for testing datasets was the best predictive model for the TBM AR. In another study, Zhou, Bejarbaneh, et al. (2020) produced ANN and genetic programming models for predicting the TBM AR and concluded that their genetic programming predictive model was the best among them. An R^2 value of 0.916 was obtained with testing data of the genetic programming predictive model. These results prove that the developed predictive model (i.e., BO-XGBoost) is a powerful, applicable, and practical system for predicting the TBM AR, and it can be recommended as an alternative model the area of TBM AR prediction.

4 Sensitivity analysis

Under certain rock conditions, predicting the TBM AR with high accuracy is the key to mechanical excavation in

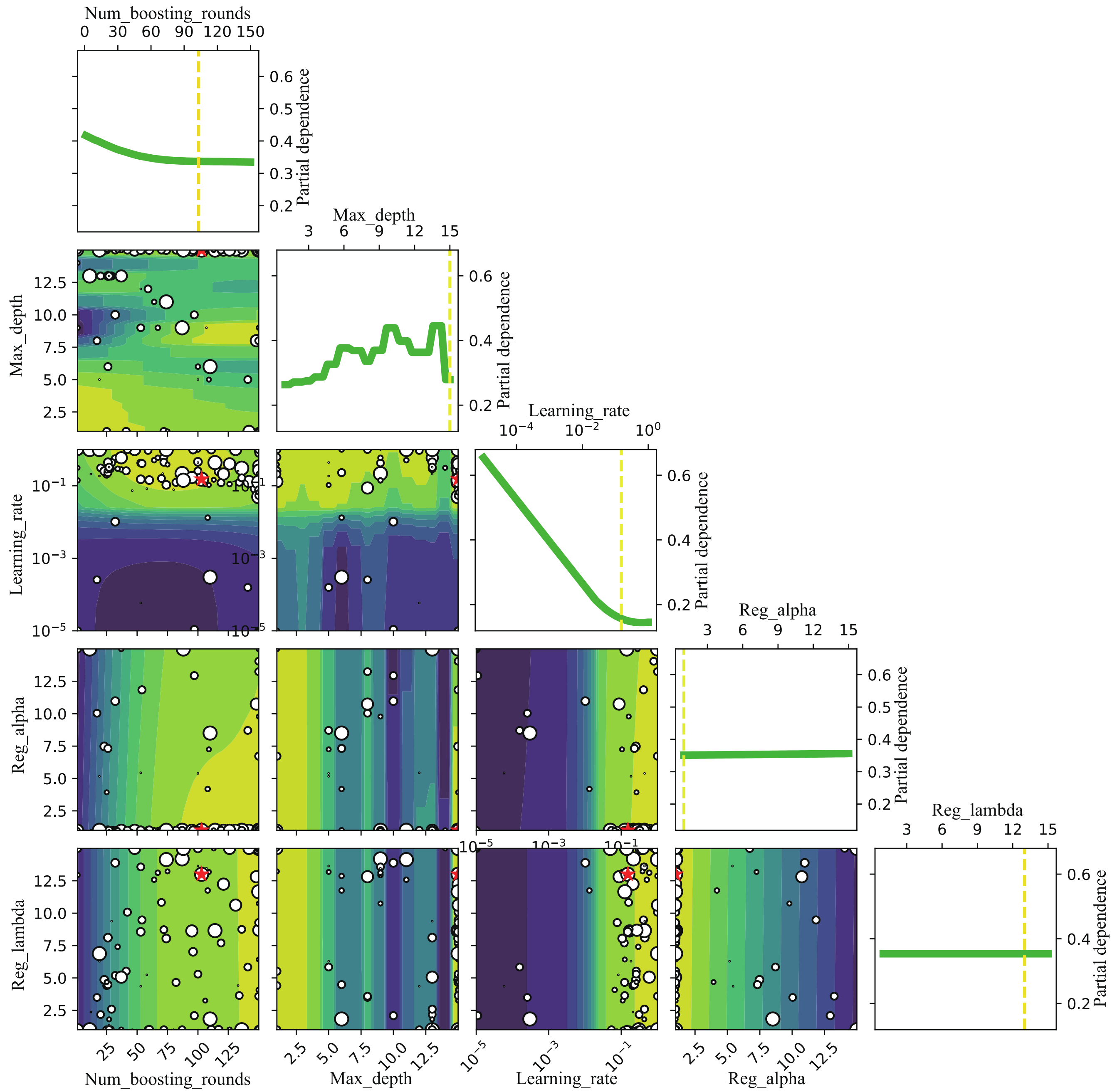


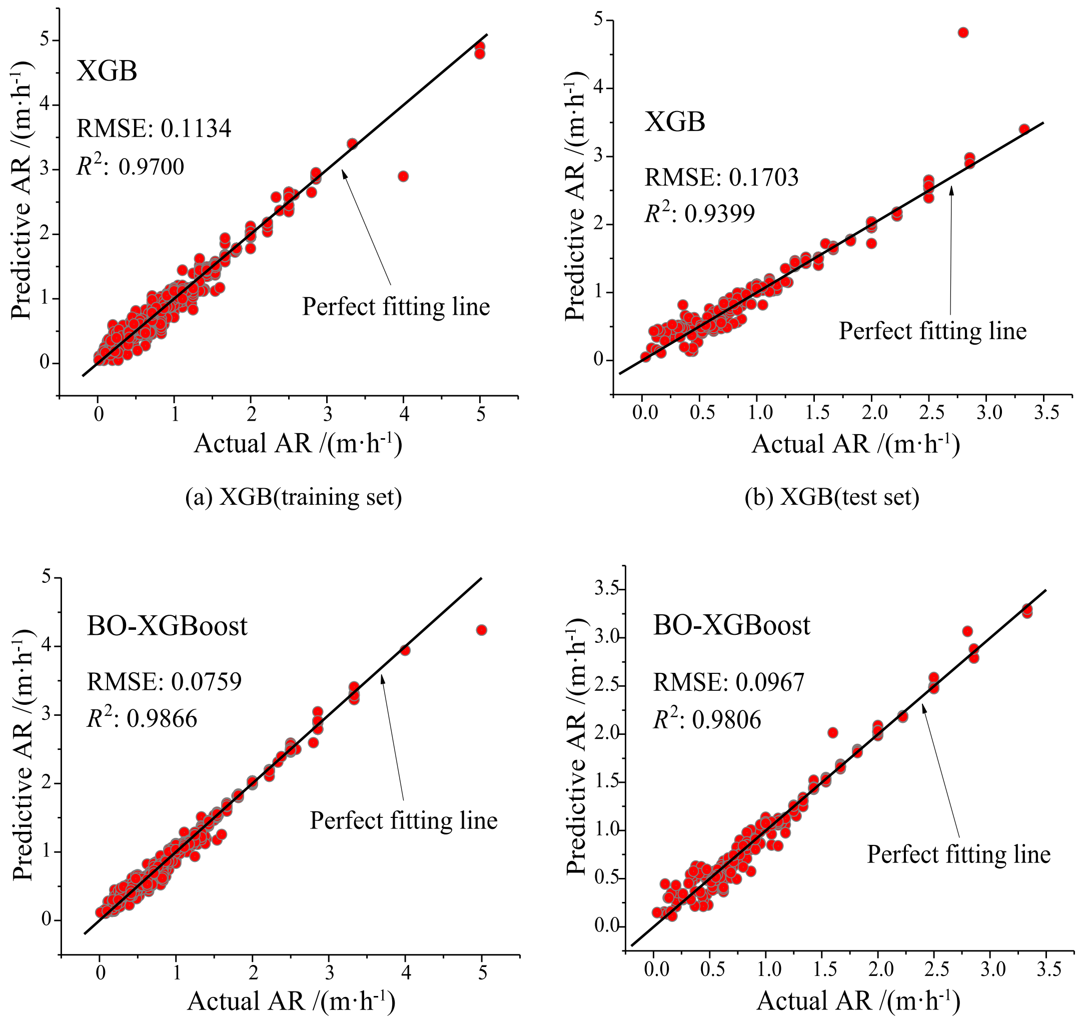
Fig. 5. Dependency plot of parameter adjustment during BO.

tunnel engineering. Various factors affecting AR must be fully considered to precisely predict the AR of TBM and reduce the high cost and risk of tunnel construction. Our study showed that all input variables (i.e., RQD, UCS, RMR, BTS, WZ, TFC, and RPM) contribute to TBM AR prediction. However, the sensitivity of each input indicator remains unclear and must be adequately resolved in further investigation.

To explore and compare the sensitivity of different factors influencing the TBM AR, the mutual information (MI) method (Verron, Tiplica, & Kobi, 2008) was used to analyze the importance of input indicators on the TBM AR. The MI method is a filtering method used to capture the arbitrary relationship (including linear and nonlinear relationships) between each feature and the label. It is a measure of the interdependence between variables and indicates the strength of the relationship between variables. The size of the MI between variables can be calculated using the information gain expressed as:

$$\mathrm{Gain}(Y,X) = \mathrm{Ent}(Y) - \sum\nolimits_{v-1}^{V} \frac{|Y^v|}{|Y|}\mathrm{Ent}(Y^v), \tag{11}$$

where v represents the number of all possible values of X, Y^v represents the set of Y corresponding to a situation when x takes x_v, and $\mathrm{Ent}(Y)$ represents the information



(a) XGB(training set)
(b) XGB(test set)
(c) BO-XGBoost (training set)
(d) BO-XGBoost (test set)

Fig. 6. Results of the XGB and BO-XGBoost models for the training and testing datasets.

Table 3
Performance comparison of the proposed BO-XGBoost and XGBoost models.

Model	Train		Test	
	R^2	RMSE	R^2	RMSE
XGBoost	0.9700	0.1134	0.9399	0.1703
BO-XGBoost	0.9866	0.0759	0.9806	0.0967

entropy. The greater the value of Gain(Y, X), the higher the correlation between X and Y.

Finally, based on the variable score from the MI method, the importance level of the input variable that predicts AR was determined. The analytical results as shown in Fig. 7 reveal that TFC, RPM, and RMR were the most important variables for predicting permeability. Their importance scores were 1.451, 1.289, and 1.040, respectively. However, it should be noted that other model inputs (i.e., BTS, RQD, and UCS) had a considerable effect on the

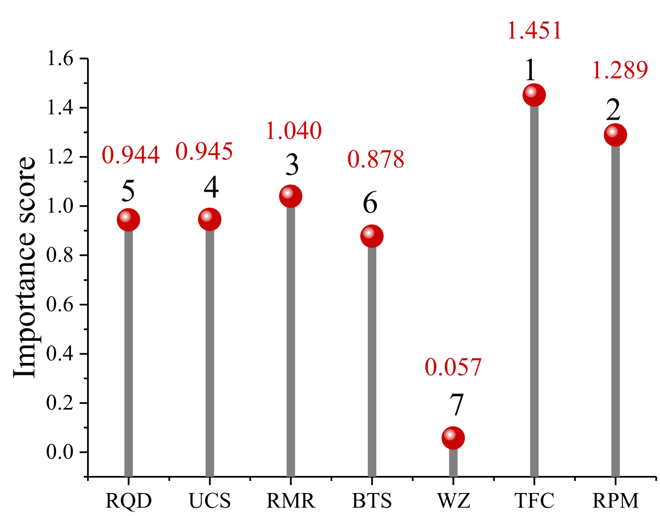


Fig. 7. Sensitivity analysis of the BO-XGBoost model with seven indicators for the TBM AR.

TBM AR. Therefore, during TBM AR prediction, TFC, RPM, RMR, UCS, RQD, and BTS are major factors to be considered. Note that WZ is not considered an influential factor for the TBM AR. For future studies, a greater number of input variables and samples must be used to enrich the dataset. This will ensure the model achieves better prediction accuracy and generalization.

5 Conclusion

The accurate prediction of TBM performance has a major influence on the smooth implementation of tunnel engineering. Therefore, this study proposed a BO-XGBoost predictive model to evaluate the TBM AR. A TBM database was created through an on-site assessment of the PSRWT tunnel project in Malaysia and related laboratory tests on samples. The TBM database contained seven input features (i.e., UCS, BTS, RMR, RQD, WZ, TFC, and RPM) and one output (AR).

By fully considering the influencing factors affecting the AR, we used the established TBM database to train and test the XGBoost and BO-XGBoost models, and RMSE and R^2 were used to evaluate the performance of the models. Finally, a variable analysis of the proposed BO-XGBoost model was performed, and the importance scores of the input variables were obtained using the MI method. There scores were 1.451 (TFC), 1.289 (RPM), 1.040 (RMR), 0.945 (UCS), 0.944 (RQD), 0.878 (BTS), and 0.057 (WZ). Of these, TFC, RPM, and RMR were considered to be highly sensitive factors.

Comparing the default XGBoost model (RMSE is 0.1703, R^2 is 0.9399) with the BO-XGBoost model (RMSE is 0.0967, R^2 is 0.9806), we observed that the BO-XGBoost prediction model was more precise than the default model, and determined that the proposed BO-XGBoost model is a reliable method for predicting the TBM AR.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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