Bayesian optimization algorithm based support vector regression analysis for estimation of resilient modulus of crushed rock materials for pavement design

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Abstract. The precise determination of the resilient modulus (MR) of the base and sub-base materials is a major preoccupation and a key criterion in the flexible pavement design process. The experimental determination of MR implies a challenging process which requires usually very difficult test procedures and extreme precautions and manpower. This is why soft computing techniques are increasingly popular and of growing importance. Many prediction techniques based primarily on linear and non-linear regression could not provide flexible use and consistent prediction of MR for practical engineering. This article introduces a hybrid of the Bayesian optimization algorithm (BOA) and support vector regression (SVR) as a new modelling tool for the MR prediction of crushed stone materials used as base and sub-base layers for pavement design. For this purpose, an experimental database was utilized to generate the hybrid BOA-SVR model of indirect estimation of the resilient modulus based on material type, basic engineering characteristics and loading conditions. The database consists of 260 experimental datasets obtained from repeated loading triaxial tests performed by the laboratory of the Central Transportation Agency located in Algiers, Algeria. To develop the model, all hyperparameters were optimised using the BOA technique. It was found that the average, median, standard deviation, minimum, maximum and interquartile range of the expected values of the developed hybrid model are very close to the experimental results. Results revealed that the hybrid BOA-SVR model predict the MR of the crushed stone materials with a coefficient of determination of 99.91% and root mean squared error of 3.55. Comparisons with traditional and other Artificial intelligence models showed that BOA-SVR hybrid model predictions are more accurate and robust than those of other models.

1 Introduction

Among the most extensive road networks in North Africa, Algeria possesses a network of secondary roads encompassing over fifty percent of its estimated one hundred thousand

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kilometres in length. In order to support the weight of traffic, these road structures typically comprise numerous unbound granular base and subbase layers in addition to thin asphalt layers [1]. The primary design parameter influencing the performance of this pavement structure is the resilient modulus of the crushed rock materials.

The Mechanistic Empirical Pavement Design Guide (MEPDG) establishes three tiers of reliability [2]. To achieve the highest tier of reliability, which corresponds to Algerian road network class 1, input from a resilient modulus test is required. However, correlations and local databases are acceptable for the second and third tiers, which correspond to secondary roads classified as medium to low volume roads and Algerian road network class 2, respectively.

As its implementation primarily relies on laboratory characterization of pavement materials and the utilisation of an extensive materials database, the Algerian Mechanistic Empirical Pavement Design Guide method [3] has encountered numerous obstacles over the past few decades. Conversely, laboratory determination of the resilient modulus of crushed rock materials is a laborious process that necessitates substantial financial investment and specialised expertise [4] due to the intricate characteristics of the materials employed in road construction. At this moment, a number of local transport agencies in Algeria lack the necessary testing capabilities to ascertain the UGMs' resilient modulus.

It is also possible to estimate the MR values of crushed rock materials (which are utilised as subbase and base granular layers in pavement construction) via predictive models. Predictive models of MR typically endeavour to establish correlations between it and various other properties, including stress state conditions [7], California Bearing Ratio (CBR) [5], liquid limit (LL), plastic limit (PL), and plasticity index (PI) [6].

The MR value of crushed rock materials can be affected by a variety of factors, including the type of aggregate, the level of stress, and fundamental properties such as unit weight, moisture content, and density [8]. Rada and Witczak [9] found that the level of stress had the greatest influence on the MR value. It was discovered that granular materials' MR tends to increase as the confining stress rises. Additionally, it has been noted that the MR of granular substances is intrinsically connected to deviator stress as a result of a change in the grain's redirection towards a denser state [10,11].

A prevalent approach among professionals is to establish relationships between the resilient modulus of crushed rock materials and various fundamental engineering properties using empirical formulas and coefficients derived from classical regression methods [12]. Nevertheless, notwithstanding their apparent simplicity, empirical methods possess several constraints. For instance, they fail to account for the extent of nonlinearity and the impact of all influential parameters. Furthermore, classical regression methods may yield weak correlations in certain empirical relationships [13].

Numerous machine learning models have been implemented in geotechnical engineering over the last few decades to forecast the complex behaviour of numerous geomaterials and establish relationships between inputs and targets of numerous experimental datasets. An examination of the specialised literature about the estimation of MR reveals that sophisticated techniques, such as artificial neural networks [14-16] and other machine learning approaches, have been utilised to construct predictive models for unbound granular substances, such as crushed rock materials [7,17].

The improvement of MR prediction model accuracy has consistently been a primary concern for numerous researchers. The utilisation of ensemble machine learning and ANN models to surpass the performance of traditional regression models has been the subject of numerous prior studies, while the application of hybrid models has been neglected.

This paper presents the development of a Bayesian Optimization Algorithm Based Support Vector Regression (BOA-SVR) model to enhance the predictive capability of the resilient modulus model.

Notably, the selection of hyperparameters is of the utmost importance when it comes to SVR. Negligible parameter selection has the potential to result in overfitting or under fitting. By integrating the Bayesian optimization algorithm (BOA) with k-fold cross-validation, SVR determines the optimal values for each of these hyperparameters.

The primary objective of this scholarly article is to calculate the resilient modulus of unbound granular substances that are commonly employed as subbase and base materials in Algeria's northern region. Mean Absolute Error (MAE), Coefficient of Determination (R^2), and Root Mean Squared Error (RMSE) are typical performance indicators utilised to assess the hybrid BOA-SVR model. The proposed model was developed utilising data from 260 experimental results stored in a local database. The outcomes of the simulations demonstrate that the hybrid BOA-SVR model accurately predicts the resilient modulus of granular materials that are not bound. Furthermore, upon comparison with alternative models including the conventional Multi Linear Regression (MLR) and the Random Forest (RF) models, it becomes evident that the hybrid BOA-SVR model exhibits superior performance across the board.

2 Materials and methods

The current investigation is conducted according to the suggested methodology, which consists of three primary phases: (1) preparation of the data, (2) development of the model, and (3) validation of the proposed model. The data acquired from laboratory tests is utilised to generate two datasets—the training and testing datasets—during the initial phase. The initial dataset is constructed using 80% of the overall data, while the subsequent dataset is comprised of 20% of the residual data. When developing the hybrid BOA-SVR model, consideration is given to the training dataset. At this stage, an investigation is conducted into the impact of hyperparameter values on the accuracy of the hybrid model. During the third stage, the testing dataset is utilised to assess the performance of the proposed model in comparison to established Artificial Intelligence models like MLR and Random Forest. Utilized statistical indicators consist of R^2, RMSE, and MAE.

2.1 Processing of data

Numerous variables impact the resilient modulus (MR) of crushed rock materials. As a means of simplifying the model, this investigation will concentrate on the primary variables that have a substantial impact on the resilient modulus.

The hybrid (BOA-SVR) model is employed to indirectly estimate the resilient modulus of crushed rock materials by utilising an experimental database. This model takes into account material type, fundamental engineering characteristics, and loading conditions. 260 experimental datasets derived from Repeated Load Triaxial (RLT) tests conducted by the laboratory of the Central Transportation Agency in Algiers, Algeria [18] comprise the database.

The RLT tests were conducted on a variety of crushed rock materials obtained from quarry crushing of three distinct types of massive rocks—granite, limestone, and diabase—which were found in various deposits situated in the northern Algerian central region.

Multiple input parameters are chosen from the experimental database, including the following: Rock Type (RT), Coefficient of Uniformity (CU), Coefficient of Curvature (CU), Fine content (Fc), Liquidity Limit (LL), Plasticity Index (PI), Maximum Dry Density (MDD), and Sample Moisture content (SMC). Additionally, two loading components are incorporated: the confining pressure denoted as σ_3 (SIGMA3) and the deviator of stress denoted (σ_d) (SIGMAD). When these parameters are utilised in modelling, the result is the resilient modulus of unbound aggregate materials (MR). [18,19] contain comprehensive

definitions and instructions on how to ascertain the input variables from laboratory tests. It is worth noting that except for the RT variable, which is categorical and accepts three values (granite, limestone, and diabase), all of these variables are numeric. The symbol, unit, and statistical analysis of the continuous variables of input and output are detailed in Table 1.

The Pearson correlation coefficient between all variables has been visualised by the correlation matrix heat map in Fig. 1.

Table 1. Statistics describing the input parameters utilised in this study

Variable	Mean	StDev	Min	Max
Cu	58.28	29.22	4.17	112.00
Cc	3.87	1.86	0.88	6.92
Fc (%)	9.46	1.99	8.00	14.08
LL (%)	28.45	4.93	19.00	37.00
PI (%)	7.08	2.61	2.00	12.00
MDD (g/cm^3)	2.23	0.07	2.11	2.34
SMC (%)	6.54	1.13	3.60	8.50
SIGMA3 (kPa)	102.85	71.34	10.00	250.00
SIGMAD (kPa)	335	160.40	150.00	600.00
M_R (MPa)	267.23	128.20	46.60	590.31

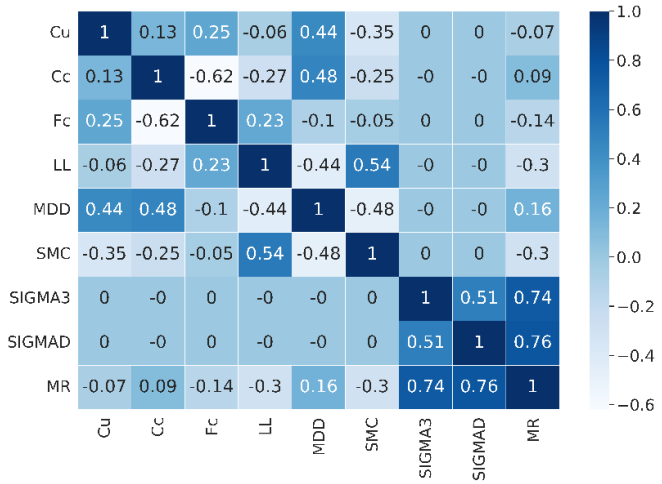

Fig. 1. Correlation matrix heat map.

2.2 Support vector regression (SVR)

The Support vector machine (SVM) algorithm is a statistical learning theory-based general classification and regression technique [21]. The utilisation of support vector regression, an extension of Vapnik's -insensitive loss function, has been implemented to address regression issues (SVR). SVR enhances its ability to generalise by employing the principle of structural risk minimization (SRM), notwithstanding its inception with a restricted set of learning data. The objective of this minimization process is to obtain a function that deviates from the actual targets by no more than ε across all training data. Due to the inevitability of errors, the objective is to restrict their occurrence to a specific range of values (ε). For nonlinear mapping, the relationship between input and output variables can be mathematically represented as equation (1) [22]:

$$k(x) = \{w.\emptyset(x)\} + b \tag{1}$$

Where x= (x_1, x_2, x_3, …, x_n) denotes the input value, y_i represents the output value and $\emptyset(x)$denotes an irregular function to assign input data to the high-dimensional domain. Furthermore, $w$represents the weight vector, which determines the orientation of a discriminating plane, $c \in R$ represents the scalar threshold, related to the bias term, and n is the size of training data. The ε -insensitive loss function is defined as [21]:

$$|y - k(x)|_\varepsilon = max\{0, |y - k(x)| - \varepsilon\}, \varepsilon > 0 \tag{2}$$

The flatness of equation (1) depends on a smaller value of w. It is practically impossible for a function to generate an error for every data point whose value is less than ε. To accommodate a greater number of errors, slack variables ξ_i , ξ_i^* are implemented. Therefore, the optimization function in SVR can be expressed as follows:

Minimize:

$$\frac{1}{2}\|w^2\| + C \sum_{i=1}^{n}(\xi_i - \xi_i^*) \tag{3}$$

subject to:

$$\begin{cases} y_i - \{w.\emptyset(x_i) + b\} \leq \varepsilon + \xi_i \\ \{w.\emptyset(x_i)\} + b - y_i \leq \varepsilon + \xi_i^* \\ \xi_i , \xi_i^* \geq 0 \end{cases} \tag{4}$$

Where ξ_i and ξ_i^* are the slack variables, b is a constant, $\emptyset(x_i)$ is a nonlinear mapping function, and C represents the penalty factor. Samples with a training error exceeding ε will be subject to a higher C value. ε specifies the requirements for the regression function. By converting the optimization problem described in equation (3) to a dual formulation utilising Lagrange multipliers, the solution can be expressed in the following final form:

$$-\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}(\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*)\, k(x_i , x_j) - \varepsilon \sum_{i=1}^{n}(\alpha_i - \alpha_i^*) + \sum_{i=1}^{n} y_i \,(\alpha_i - \alpha_i^*)$$

Subjected to:

$$\sum_{i=1}^{n}(\alpha_i - \alpha_i^*) = 0;\ \alpha_i , \alpha_i^* \in [0 , C] \tag{5}$$

Where: $k(x_i , x_j) = \emptyset(x_i).\emptyset(x_j)$ is defined as the kernel function

Upon resolving equation (5) for the given values of α_i, α_i^*, equation (1) can be expressed in its final form as follows:

$$k(x) = \sum_{j=1}^{n}(\alpha_i - \alpha_i^*)\, k(x , x_i) \quad + b \tag{6}$$

Radial Basis Functions (RBFs), sigmoid, linear, polynomial, and Fourier series functions are the most prevalent kernel functions. The present study employed the RBF function, which is defined as follows:

$$k(x, x_i) = e^{(-\gamma \|x - x_i\|^2)} \tag{7}$$

Where γ is the kernel parameter. In addition, the prediction accuracy of the SVR using the RBF kernel is contingent upon three parameters ε , γ and C.

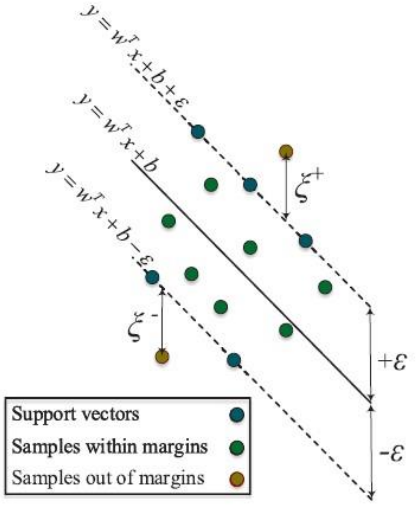

Fig. 2. A graphical depiction of support vector regression.

2.3 Bayesian optimization algorithm (BOA)

The BOA is based on Bayes' rule, as shown in equation (8) below [23]:

$$p(w|D) = \frac{p(D|w)\, p(w)}{p(D)} \tag{8}$$

Where w represents an unobserved value, p(w) represents the distribution preceding it, p (D| w) represents the probability, and p (w| D) represents the posterior distribution. Bayes' rule incorporates prior knowledge to ascertain the posterior possibility; thus, the outcomes of previous iterations will be utilised in determining the values for the subsequent iteration. Consequently, it approaches the optimal point with greater efficiency than arbitrary selection. The BOA applies to both the acquisition and the substitute sub-models. The objective function is assessed by the substitute model utilising the Gaussian process (GP), a widely accepted alternative for simulating the objective function.

The following is an expansion of the Gaussian distribution. In general, GP establishes a prior over function which can be transformed into a posterior over function after the observation of certain function values.

As illustrated below, this technique, the function $f\ (x)$ is assumed to be a realization of GP with the mean function $m\,(x)$ and the covariance function $k(x, x_i)$, where x is the function value with any potential pair of (x_i, x_j) in the input domain. Additional information can be found somewhere else [24]:

$$f(z) \sim GP(m\,(x)\,, k(x_i, x_j) \tag{9}$$

Each input parameter in this function represents a variable that is interconnected with other variables defined in the input domain, including those outlined by the covariance function. As a kernel, the covariance function regulates the amplitude and smoothness of the Gaussian process samples. Conversely, the BOA's acquisition function is optimised through repetitions and is dependent on prior observations. The subsequent iteration point is proposed by the acquisition model based on the outcomes of the substitute model. The mathematical representation of hyperparameter optimization utilising BOA is denoted by equation (10):

$$\overset{*}{g} = \arg\min_{g \in G} f(g) \tag{10}$$

Here, $f(g)$ is the objective score to reduce root mean square error (RMSE), $\overset{*}{g}$ is the set of hyperparameters that generates the lowest value of the score, and $\overset{*}{g}$ is any value of space G. BOA was utilised in this study because it is more effective than other available optimization methods (e.g., grid, random search, manual, particle swarm optimization). Additionally, it facilitates the systematic optimization of black box functions on a global scale [25,26].

The optimization of the hyperparameters (ε, C, γ, kernel function) is achieved through the integration of the SVR algorithm and the Bayesian optimization algorithm (BOA). Before the BOA was implemented, the k-fold cross-validation method was employed. The train data are succinctly divided into k subsets in the same manner. A test subset is selected from one dataset, whereas the remaining subsets are utilised for training purposes. By iterating this method k times, each subset is utilised precisely once for the test. The optimization algorithm comprises the subsequent stages:

1. Configuration of SVR model hyperparameters for the kernel function, ε, C, γ
2. Set the objective function
3. Develop a surrogate probability model of the objective function
4. Determine the optimal hyperparameters for the surrogate model.
5. Apply the following hyperparameters to the actual objective function:
6. Incorporate the new result into the surrogate.
7. Repeat the step 3 to 6 until the maximum number of trials is reached
8. Determine the optimised hyperparameters
9. Employ these optimised hyperparameters in the construction of the SVR model.

2.4 Statistical indices

Three statistical indices were employed in the present study to evaluate the performance of the proposed models. The mean absolute error (MAE) quantifies the discrepancy between the predicted and measured MR values. To determine the average magnitude of the errors, RMSE was applied with greater significance to larger errors. The precision of the predicted MR values was assessed using the coefficient of determination (R^2). Comprised of the subsequent equations are the statistical indices:

$$MAE = \frac{1}{N}\sum_{i=1}^{N}|y_i - t_i| \tag{11}$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - t_i)^2} \tag{12}$$

$$R^2 = \left(\frac{\sum_{i=1}^{N} (t_i - \bar{t})\,(y_i - \bar{y})}{\sqrt{[\sum_{i=1}^{N} (t_i - \bar{t})^2]\,[\sum_{i=1}^{N} (y_i - \bar{y})^2]}} \right)^2 \quad (13)$$

Where y_i and t_i are predicted and measured values, $\bar{y}$ and $\bar{t}$ are the mean of the predicted and measured values of M_R respectively, and N denotes the number of data records.

3 Results and discussion

3.1 Development of a hybrid BOA-SVR model

The development of the BOA-SVR model involves the adjustment of its hyperparameters (specifically, the kernel function, C, ε, γ), as these parameters significantly impact both the accuracy of the model and the computation time. The literature contains numerous well-known methods for tuning hyperparameters, including the random search algorithm, the grid search algorithm, particle swarm optimization, and the Bayesian optimization algorithm (BOA). It is noteworthy to mention that both the random search and grid search algorithms necessitate numerous iterations and can be laborious. Particle swarm optimization is a time-consuming and well-known conventional method. The BOA, on the other hand, is a cutting-edge optimization framework that determines the optimal parameters significantly faster than the alternatives by utilising an acquisition function that computes the subsequent point to evaluate. The BOA was chosen for the current study as it is a methodical adjustment procedure that obviates the necessity for derivatives [26,27]. Furthermore, it yielded superior outcomes in comparison to alternative approaches.

To prevent overfitting, a 10-fold cross-validation strategy was selected due to its low root mean square error (RMSE) and computational time of 34.85 seconds. BOA was utilised to optimise the kernel function type, epsilon, box constraint, and kernel scale values; the predictive accuracies of the models were then evaluated. The optimal point of the SVR hyperparameter optimization process is depicted in Fig. 3. The minimum observed objective score of 7.90 was recorded across 79 trials (iterations). The determination of the optimal model utilising the tuned parameters as specified in Table 2 was based on the precision level.

Table 2. The optimized parameters for the used SVR model

Parameters	Range/type	Optimized parameters
Kernel function	RBF, Polynomial	29.22
Epsilon	$[10^{-5},10^{5}]$	0.000153
Box Constraint	$[10^{-5},10^{5}]$	9154.00
Kernel Scale	$[10^{-5},100]$	0.0754

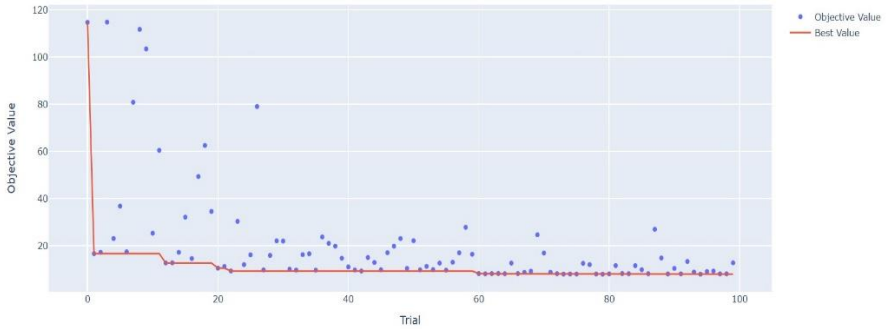

Fig. 3. The progress of Bayesian hyperparameters optimization.

In light of the data-dependent nature of intelligence-based models, the applied BOA–SVR model was developed through empirical laboratory experiments. Significantly, both experiments and the SVR model were utilised to generate descriptive statistics and distribution of results. The statistical analyses of the measured and estimated values of the resilient modulus using the BOA-SVR model are presented in Table 3.

Table 3. Statistical summary of the measured values and the BOA–SVR model predictions

Parameters	Measured	BOA-SVR
Mean	303.12	302.90
Std. Deviation	126.08	125.59
Min	102.46	102.72
Max	590.31	586.77

A common method for illustrating the distribution of data through a five-number summary, including the median, minimum, and maximum scores, as well as the first and third quartiles, is the use of a boxplot. The boxplots of experimentally determined and predicted resilient moduli of crushed rock materials are displayed in Fig. 4. The findings indicate that the predicted and measured output distributions were similar.

Due to the fact that each median line is enclosed within a box, there was no discernible distinction between the datasets. The absence of substantial variability in the interquartile ranges for both the assessed and anticipated values indicates that the findings may not have been widely disseminated.

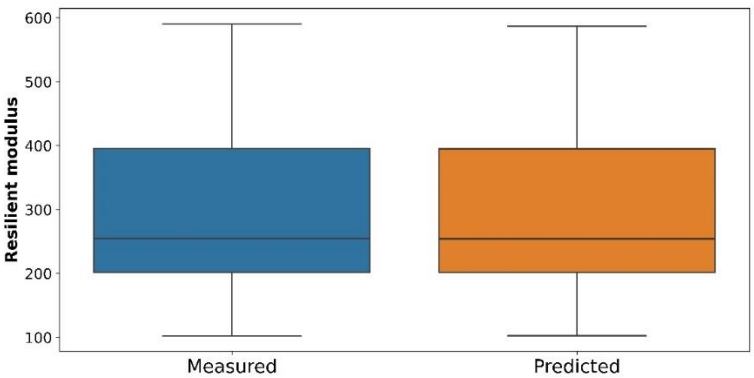

Fig. 4. Box plot for measured and predicted resilient modulus.

3.2 Assessment of the BOA-SVR hybrid model

Utilizing the hybrid BOA-SVR model that was created for this investigation, the resilient modulus of crushed rock materials was estimated. The fitted line, denoted as the 45◦ line, illustrates the relationship between the experimental and model-predicted resilient moduli in Fig. 5. The fitted line is obviously in close proximity to the 45° line. The fitted curve on the test dataset exhibits a coefficient of determination (R^2) of 99.92 percent, signifying a satisfactory level of fit. Thus, it can be asserted that the predicted outcomes closely resemble the data obtained in the experimental laboratory. Automatic hyperparameter tuning was employed to optimise the model's performance in proximity to the experimental data. Additionally, k-fold cross-validation was utilised to mitigate the risk of overfitting. As a result, improved forecasts were attained.

Furthermore, to evaluate the model's compatibility, Fig. 6 displays the outcomes of residual analyses. Notably, the residual plot resembles a scatter plot; the model is acceptable if residual data points are dispersed around the zero line. It is noteworthy that Fig. 6 illustrates that every residual data point is observed near the zero line. This observation provides further support for the model's reliability and validity.

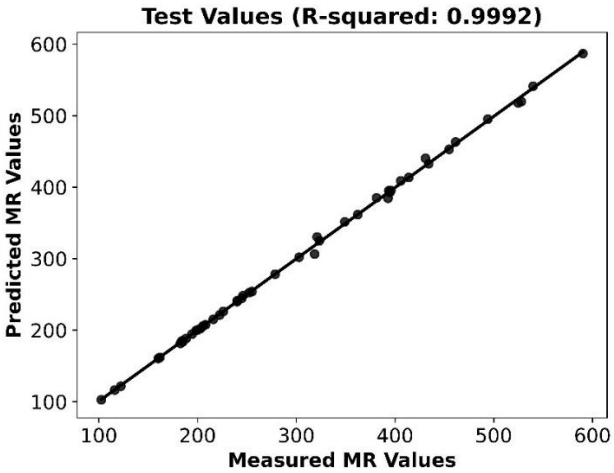

Fig. 5. Measured and predicted values plotted with a fitted line.

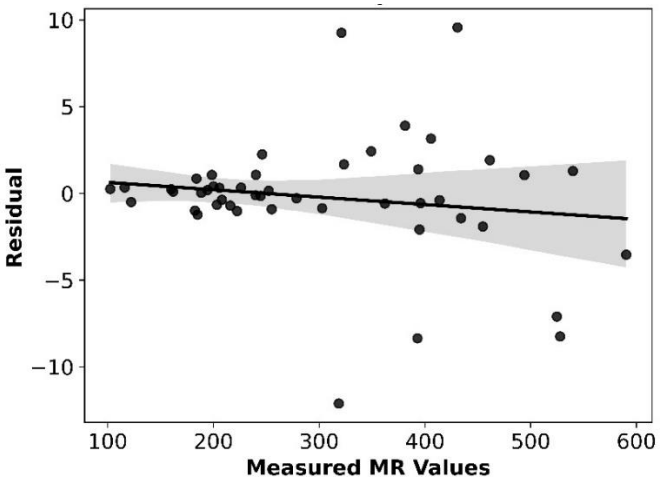

Fig. 6. Residual plot.

It was observed that every statistical error parameter (MAE, RMSE) was minimal. Based on the findings presented in Table 4, it can be concluded that the predictive model employed in this study for the resilient modulus of crushed rock materials is highly satisfactory. Notable is the fact that predictions generated by the hybrid BOA–SVR model are deemed reliable when the error and coefficient of determination values approach zero and one, respectively. The SVR model undoubtedly meets this particular criterion.

Table 4. Performance indices for training and testing dataset

	Train data	**Test data**
MAE	0.21	2.07
RMSE	0.64	3.55
R^2	0.9999	0.9992

3.3 Analysis of the hybrid model's performance in comparison to other artificial intelligence models

To facilitate a direct comparison between the BOA-SVR model and established other Artificial Intelligence models, every performance metric derived from the hybrid model is assessed in relation to conventional MLR and Random Forest models. In Table 5, the MAE, RMSE, and R^2 values are compiled.

Table 5. Comparison of model performance on the test dataset

	BOA-SVR	**MLR**	**RF**
MAE	2.07	22.78	27.33
RMSE	3.55	26.40	36.16
R^2	0.9992	0.9300	0.9024

As anticipated, the results presented in Table 5 demonstrate that the hybrid BOA-SVR model significantly outperformed the MLR and RF models, as indicated by its significantly lower MAE and RMSE and higher R^2.

4 Conclusion

A support vector regression model based on a Bayesian optimization algorithm was developed in this article to estimate the resilient modulus of crushed rock materials. Cross-validation was performed tenfold in order to prevent overfitting. The BOA-SVR model was developed utilising an extensive collection of 260 experimental datasets collected by the laboratory of the Central Transportation Agency on crushed rock materials. The evaluation of the model's performance was conducted by employing various indicators for measuring performance. A comparison was also made between the predicted outcomes and conventional Artificial Intelligence (AI) models. Based on the outcomes of the simulations, the subsequent deductions can be made:

1. The experimental results and the estimated resilient modulus of crushed rock materials using the hybrid BOA–SVR model are remarkably congruent. Furthermore, the interquartile ranges, means, medians, and standard deviations of the predicted and measured outcomes are extremely similar.
2. The estimated results and laboratory results are in agreement due to the extremely close proximity of the R^2 value between the measured and predicted values to 1.
3. The residual data points of the proposed model are observed to be around the zero line, providing additional confirmation of the model's dependability.

4. In contrast to the alternative artificial intelligence models discussed in this paper, the BOA–SVR model exhibits the smallest mean, standard deviation, and coefficient of variation.
5. Particularly for roads with low to moderate traffic volume, a dependable soft computing tool for pavement design can be constructed using the BOA–SVR model.
6. Since the proposed model is constructed utilising a regional database, augmenting its generalizability with supplementary data from other areas could be beneficial.

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