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Research Article

Analysis of Marshall's Stability of Hot Mixtures with Machine Learning

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Keywords

Asphalt concrete,
XGBoost,
Machine learning,
Marshall stability,
SHAP.

Abstract

Road transport is the most widely used transport network globally and in Turkey. Every year, asphalt mix designs are prepared for the deterioration or reconstruction of road pavements. Since asphalt mixture designs affect the mechanical and physical properties of roads, they also directly affect their performance. For this purpose, Marshall design, one of the experimental methods, is used. The calculation of design parameters used in mixture design is complex, time consuming and costly. To address this, developing models that predict experimental results using machine learning methods offers an economical and practical approach. A data set consisting of 13 variables including specific gravities, aggregate proportions and bitumen content was created for 453 hot mix asphalt specimens subjected to the Marshall test. Marshall Stability (MS) was determined as the target variable in the model. Random Forest, XGBoost, GBoost and Extra Trees algorithms were used to predict MS; models were compared with performance metrics such as MAPE, R^2 and RMSE. The XGBoost model was the most successful model for MS prediction; it provided high accuracy and low error rate with R^2 (coefficient of determination) of 0.96, RMSE (root mean square error) of 0.37 and MAPE (mean absolute percentage error) of 0.02% on the test data. SHAP analysis was performed to determine the variables affecting MS prediction, and the most effective variables were found to be Gef (effective specific gravity of aggregate) and Gsb (bulk specific gravity of aggregate). Such explainability analyses facilitate decision making in the early design stages by supporting the optimization of design parameters.

1. Introduction

In the globalizing world, transportation has become an indispensable part of both individual and social life; therefore, interest and demand for transportation has increased day by day. Today, 90.6% of freight transportation and 90.9% of passenger transportation in Turkey is done by road [1]. Considering that increasing traffic density affects the performance of the superstructure, road construction is given considerable importance. In order to prevent the deterioration of the superstructure coatings, mixture designs that will not require maintenance and repair for a long time are required [2].

Mixtures obtained by combining bitumen and aggregate in appropriate proportions are used as road pavement in the form of surface coating or HMA mixture depending on the application method. In addition, HMA mixtures are one of the most widely used pavement types as they provide durability, driving comfort, stability and high resistance to water permeability. While the aggregate used in these mixtures provides internal friction resistance, bitumen affects the mechanical properties of the mixture by increasing the cohesion strength. HMA mixtures are generally designed to contain 95% aggregate and 3-7% bitumen. Therefore, great care must be taken in the selection of aggregate, as it will directly affect the performance of the mixture. Especially in road construction, deteriorations such as abrasion and wheel tracks are mostly due to wrong aggregate selection [2-3]. In addition, in order for the performance of HMA mixtures to be at the desired level, optimum bitumen content should be used. Adjusting these ratios requires optimizing mix designs. Therefore, Marshall test is generally used when preparing HMA mixtures [4]. In Marshall design, aggregate gradation and optimum bitumen content criteria affect the design parameters. Aggregate gradations are categorized into three types: open (characterized by larger voids and poor interlock), dense (well-graded with minimal voids and high stability), and average (a mid-range gradation with intermediate characteristics between open and dense). In the studies conducted, it was observed that the mixtures used in average gradation curves increased stability. Although the highest stability was obtained with the average gradation, it was also observed that the decrease in the maximum total size of the aggregate increased the stability. In another study, coarsening or finening of aggregate gradation decreased Dp (Bulk Specific Gravity of Mixture) and Vf (Voids Filled with Bitumen) values and increased VMA (Voids in Mineral Aggregate) and Vh (Air Voids) values [5].

In Marshall design, more than one experiment is performed to improve the HMA mixture properties and to find the most appropriate design parameters. This situation is costly in terms of engineering [6]. With the advancement of technology, solutions using machine learning models began to be investigated. Studies have shown that the properties of superstructures can be evaluated by various methods. In a study, adaptive neuro-fuzzy inference system (ANFIS), multiple expression programming (MEP) and artificial neural networks (ANN) methods were applied to estimate MS and MF (Marshall flow) variables using 343 data points. As a result of the modeling performed using Marshall design parameters, the MEP method with an R^2 value above 90% showed better performance than other models) [7]. In another study, MEP method was applied to estimate MS and MF variables using data from road projects in Pakistan. Modelling based on Marshall design parameters resulted in low error and high accuracy (R^2 > 90%) based on R^2, RMSE and MAPE criteria [8].

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In the study, experimental data of 453 different asphalt mixture samples prepared under laboratory conditions were taken from the thesis study [9]. After analyzing these data, the Lazy Predict library was used for model selection and the performances of various machine learning algorithms were compared. The Lazy Predict method offers the opportunity to propose different regression models in a short time by writing a very small amount of code. The main models proposed in this study include GBoost, XGBoost, Random Forest and Extra Trees algorithms [10]. The main purpose of this study is to estimate the Marshall Stability (MS) value defined as the target variable. To achieve this, the performances of the selected models for MS prediction were compared using statistical metrics. According to the evaluation results, the model that showed better performance in estimating the MS value was the XGBoost algorithm. The XGBoost model exhibited better prediction performance compared to other machine learning algorithms with its superior R^2 score (0.96), low RMSE value (0.37) and very low MAPE ratio (0.02%) on the test data. However, SHAP analysis was performed to interpret the effect of input parameters on the estimated MS value. Among the variables, Gef and Gsb exhibited the most significant influence on the estimated MS value. However, predictability of design variables is of great importance for sustainable and economical road designs. In this context, information on the data set, method and analysis processes used in the study are explained in the 'Materials and Methods' section.

2. Materials and Methods

This section describes the data collection stages. After the dataset was subjected to pre-processing steps such as cleaning outliers, scaling features, removing missing data, and applying necessary data transformations, the machine learning techniques to be applied were determined. Modelling based on Marshall design parameters resulted in low error and high accuracy ($R^2 > 90\%$) based on R^2, RMSE and MAPE criteria. The flow chart of this process is given in Figure 1 [11].

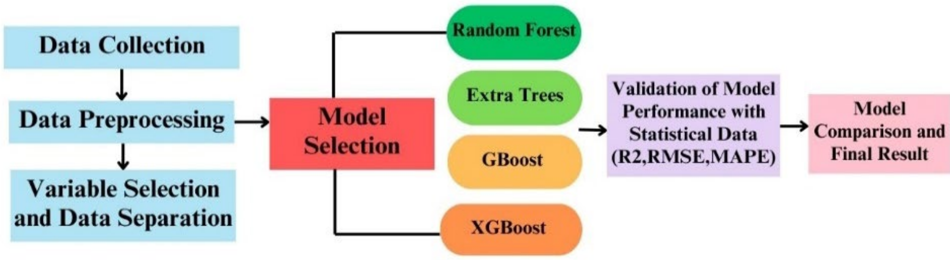


Figure 1. Workflow diagram of machine learning techniques in practice

2.1. Data Collection and Pre-Processing

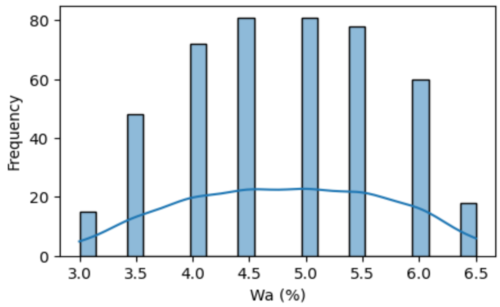
In this study, design data of a total of 453 asphalt mixture samples were collected for abrasion, binder and bituminous base layers obtained under laboratory conditions. The data were obtained from cylindrical samples prepared according to the ASTM D 6927 Stability and Flow Method of Marshall Asphalt Mixtures standard used for the road project. In addition, the standards specified in Highway Technical Specification (HTS) 2013 Section 407 Asphalt Concrete 'Binder', 'Abrasion' and 'Bituminous Base Course' were taken into consideration for the design mixtures in the study [12]. A total of 13 input parameters were used in the modeling considering Gef, Gsb, Pb (Bitumen Content), Wa (bitumen-aggregate ratio by weight), bitumen penetration, CA/FA, F/B, Dmax, Dp, Dt (theoretical maximum density of the mixture), VMA, Vh and Vf. MS was used as the output parameter. The IQR method was used to detect outliers in the input and output parameter values. With this method, outliers were identified and the data was cleaned. Then, the data set was standardized using the Standard Scaler function from Scikit-learn. Thus, the accuracy of the model was increased [11]. Statistical information regarding the data prepared accordingly is presented in Table 1.

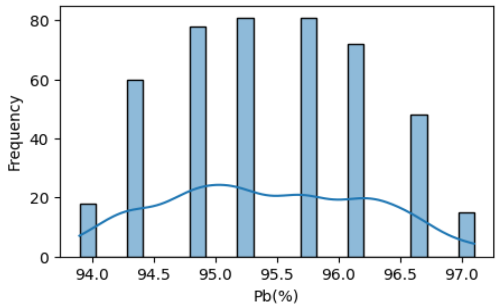
Table 1. Statistical information about the dataset

Parameters	Sample Size	Mean	Standard Deviation	Min	25%	50%	75%	Max
Bitumen Penetration (mm)	453	70.13	9.83	59	62	63	82	88
Gef (gr/cm3)	453	2.71	0.08	2.522	2.681	2.704	2.775	2.824
Wa (%)	453	4.80	0.90	3	4	5	5.5	6.5
Pb (%)	453	95.42	0.83	93.9	94.8	95.2	96.2	97.1
Gsb (gr/cm3)	453	2.68	0.08	2.471	2.644	2.68	2.739	2.768
Dp (gr/cm3)	453	2.39	0.07	2.197	2.356	2.42	2.441	2.497
Dt (gr/cm3)	453	2.52	0.07	2.332	2.478	2.529	2.572	2.676
Vh (%)	453	5.06	1.86	1.05	3.76	4.79	6.39	9.72
V.M.A (%)	453	14.60	0.93	12.23	14.04	14.61	15.17	17.24
Vf (%)	453	65.29	12.82	32.03	55.93	66.9	74.9	92.21

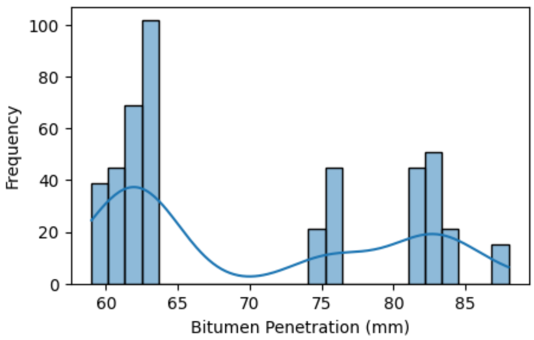
Dmax(mm)	453	26.67	7.44	19.1	19.1	25.4	37.5	37.5
CA/FA	453	1.44	0.16	1.2	1.3	1.5	1.6	1.8
F/B	453	1.09	0.24	0.6	0.9	1.1	1.2	1.9
MS (kN)	453	12.00	1.85	6.15	11.25	12.43	13.31	15.12

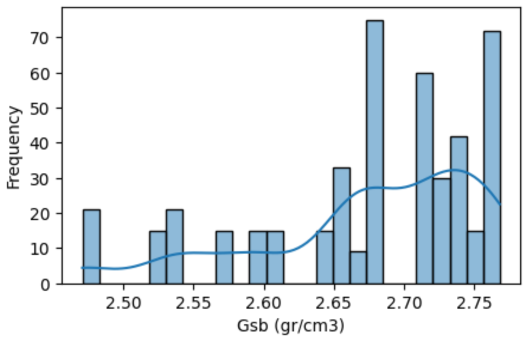
Figure 2 shows the frequency plots of the data set. Graph (a) shows that the Wa variable increases steadily between 3-6.5% and similarly, graph (b) for the Pb variable shows a comparable distribution between 94-97%, consistent with the literature [3]. Graph of the bitumen penetration variable (c) shows a multimodal distribution, probably due to the inclusion of different grades of bitumen. Climatic conditions are taken into account when determining bitumen classes [13]. When (d) and (e) graphs of the aggregate are analyzed, different peak distributions for Gsb and Gef properties, respectively, indicate that the aggregates have different physical properties (e.g. porosity, water absorption content, etc.) [14]. Graph (f) of the CA/FA (coarse aggregate/fine aggregate) variable shows that while a high coarse/fine ratio generally improves stability, an excessive increase can have a negative effect, emphasizing the need for optimum ratios [15]. The graph of the F/B variable (g) shows that the highest frequency is at a value of 1. Here, the F/B ratio is desired to be between 0.8-1.6. If the F/B ratio is too low, it causes lateral displacement during compression. If it is too high, it causes stress cracks [16]. It has been observed that the graph of the Dp variable (h) of the mixture is also skewed to the right. This feature allows us to understand the performance of the mixture [17]. In the graph of the Dt variable (i), there is a distribution of different values, which indicates that different types of aggregates or mixtures are used in the mixture [18]. Similarly, the Vh variable (j) graph shows that it affects moisture damage and stability since its different values are found to be in a wide range [19]. Looking at the graph of the VMA variable (k), a uniform distribution is observed and the highest frequency is observed at an average value of 15%. If the VMA value is too low, the stability is low due to the thin layer of bitumen between the aggregates [5]. The (l) graph for the Vf variable shows the highest frequency close to 70%. For the Dmax variable, the graph (m) shows three different peak values. The graph of the target variable MS (n) shows a regular distribution.



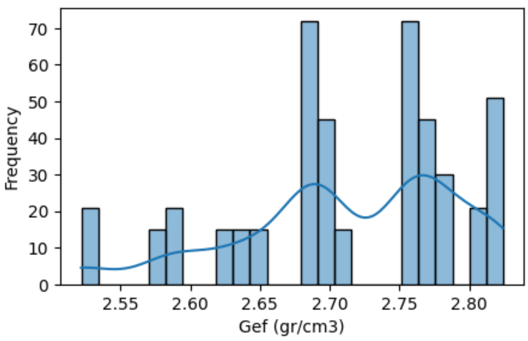


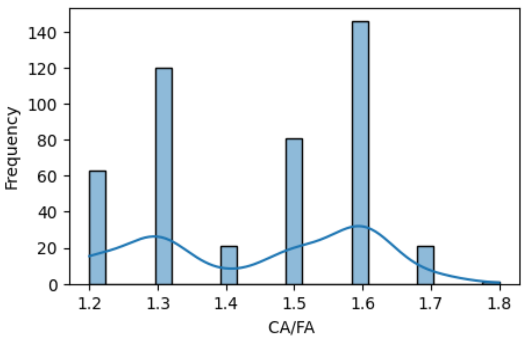
(a) (b)



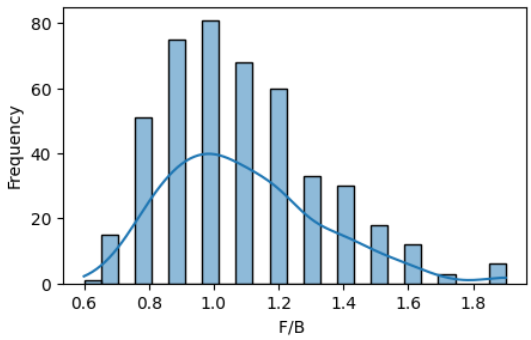


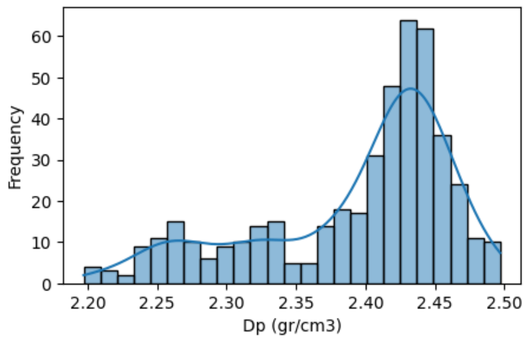
(C) (d)



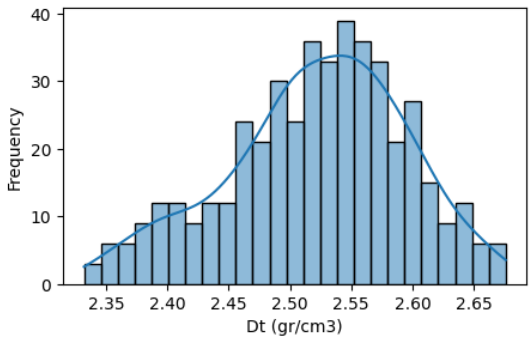


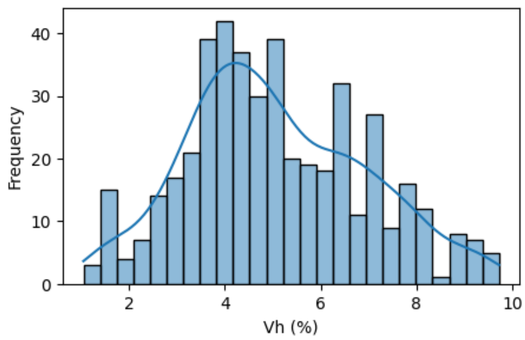
(e) (f)



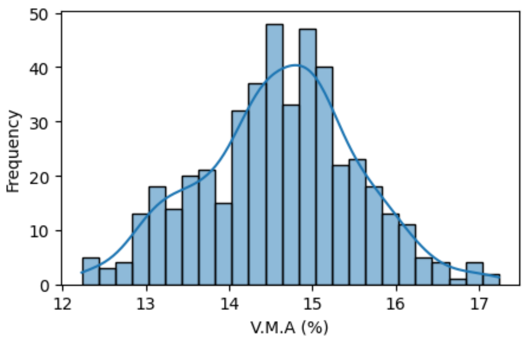


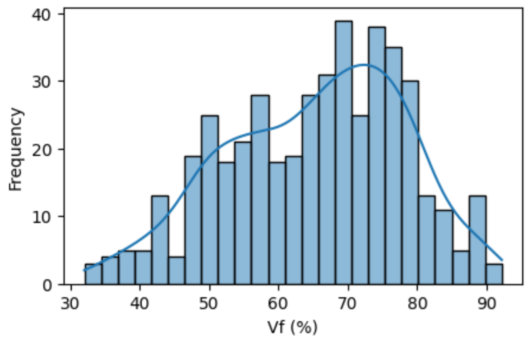
(g) (h)



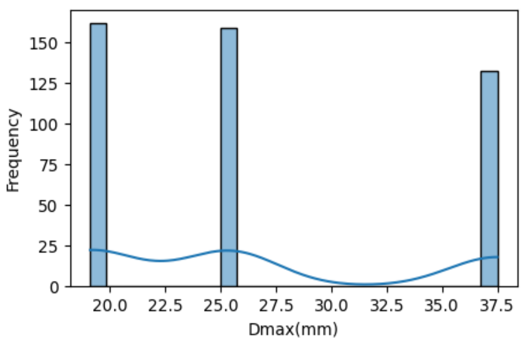


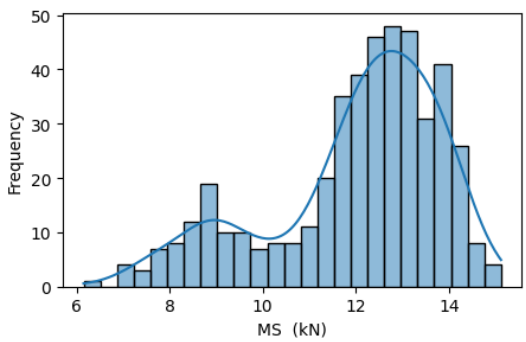
(i) (j)





(k) (l)





(m) (n)

Figure 2. Frequency distribution graphs of the data set

2.2. Variable Selection and Data Separation

For the estimation of the MS value using the collected data, it is known that the correlation between variables can affect the performance of non-tree-based models. However, in tree-based models, since the variables form a decision structure by branching within themselves and only the variables that provide the highest information gain are selected as partition criteria, the correlation relationship between them does not have a significant negative effect on model performance [20-21]. After the variables to be included in the study were determined, some of them were reserved for training and some for testing, depending on the size of the data set. In cases where the data set size is limited, it is recommended that 80% of the data be used for training the model and the remaining 20% for testing, as a common practice [22]. Accordingly, the data were used at an 80/20 ratio.

2.3. Selection and Analysis of Models

The Lazy Predict method in the sklearn library was used to determine which machine learning technique to use in the datasets. Thus, minimal code was written and as a result, the analyses were carried out in a practical way. As a result of the analysis, it is recommended to use the models with the highest accuracy rate and the lowest error rate [10]. Here, the first 4 models recommended in the Lazy Predict method are Extra Trees, XGBoost, GBoost and Random Forest algorithms, respectively. Explanations for these models are provided below.

Random Forest: Within the scope of the Random Forest method, the data set was first divided into training and test subsets. Then, the training data was randomly divided into subsets using the bootstrap method. This method aimed to increase the generalization performance of the model by increasing the independence between the data. Decision trees were created by randomly selecting samples from each subset. These trees were trained without pruning and prediction results were obtained [23-24].

Extra Trees: The Extra Trees algorithm works with a similar logic to the Random Forest algorithm. However, Extra Trees algorithm creates decision trees with a different method. At this stage, the dataset was divided into training and test subsets. In the process of creating decision trees, the training data was prepared directly using the original samples without any resampling. Each decision tree selects a random feature at its node and makes random splits on this feature. This method increases the variance by reducing the correlation between decision trees [25].

GBoost: GBoost usually starts with an initial estimate (e.g. average) and then builds trees to estimate residuals (errors)For this purpose, the average of the variable column to be estimated is taken. The first tree builds a predictive model based on these error rates. Thus, decision trees begin to be created. Learning rate is applied to reduce the differences in decision trees. By proceeding in small steps, the error rate is reduced and the accuracy of the test results is increased. This process continues until the trees come together to form a meaningful model [26].

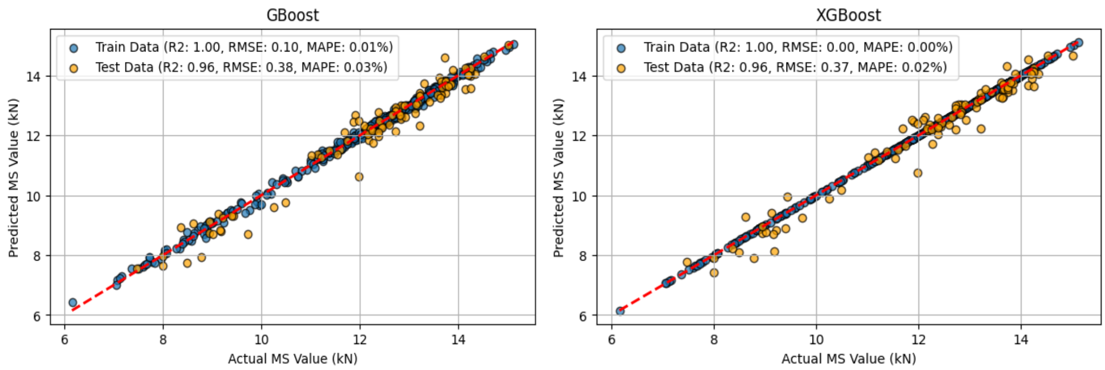
XGBoost: Similar to GBoost, it usually starts with a fixed estimate (usually the mean of the target variable). Then, the target variable is predicted repeatedly by creating decision trees, similar to the learning technique in GBoost. A similarity score (Gain score) is calculated for the branches of each decision tree. This score indicates how well the branches are divided. Pruning is applied during tree construction to prevent overfitting. The pruning process is evaluated using the gamma parameter. If the gamma value is greater than the gain score, the relevant branch is pruned, so that only the branches with high scores are preserved and overfitting is prevented. This process continues until the errors in the tree are corrected and the model becomes meaningful [27]. Thus, model selection is performed. Performance is increased by performing hyperparameter optimization for each model separately [10]. In order to improve the performance of the model selections determined in the study, the most appropriate hyperparameter for each model was optimized with the proposed grid search and random search [11]. In this way, high performance was achieved by training the model. The appropriate hyperparameter values in this study are presented in Table 2.

Table 2. Hyperparameter values used for machine models

	Marshall Stability, MS (kN)
Random Forest	bootstrap=true, max_features=1.0, min_samples_leaf= 1, min_samples_split=2, n_estimators= 100, random_state= 95
Extra Trees	bootstrap=false, max_features= 1.0, min_samples_leaf=1, min_samples_split=2, n_estimators=100, random_state=312
GBoost	alpha= 0.9, learning_rate= 0.1, max_depth= 10, min_samples_leaf= 1, 'min_samples_split= 2, n_estimators= 120, random_state= 312, subsample= 0.3, validation_fraction= 0.9
XGBoost	learning_rate=0.2,n_estimators=300,max_depth=12,subsample=0.5,colsample_bytree=0.6,random_state= 312

3. Results and Discussions

Statistical parameters R^2, RMSE and MAPE were used to evaluate the model performance and validation. A higher value of R^2 indicates the increased accuracy of the model. However, MAPE and RMSE values approaching zero indicate models with minimum error rates and improved performance. The prediction models generated with the machine algorithms used in this study are presented in Figure 3. The y-axis of the graphs represents the predicted MS and the x-axis represents the actual MS. The dashed diagonal line (x=y) highlights the good performance of the model because when the actual values and the predicted values are in the same direction, forming a linear shape, the success of the model increases [28]. In addition, it was seen that the model with the closest R^2 value to 1 and the lowest error metric (RMSE, MAPE) is the XGBoost method. The R^2 (0.96), RMSE (0.37) and MAPE (0.02%) values of the XGBoost method on the test data show that it gives better results than the other models.



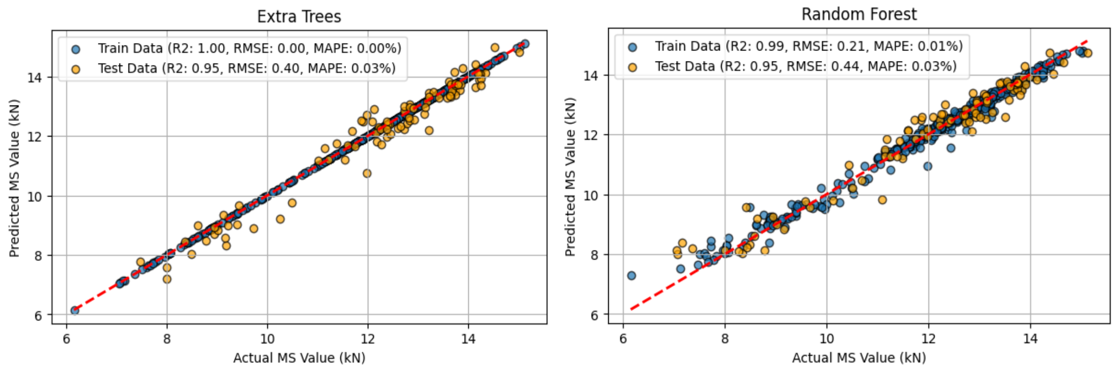


Figure 3. Predicted MS value results of the models

SHAP summary graphs of MS values for the developed models are shown in Figure 4. In these graphs, the input parameters are listed from top to bottom according to their impact levels. For all models, Gef was found to be the parameter that contributed the most to the overall prediction of the MS value. Positive values on the x-axis of the SHAP summary graph contribute positively to the prediction of the MS value, while negative values contribute negatively to the prediction. In addition, as we move from red values to blue values, the value of the data feature decreases [29]. In the XGBoost model, which performed better than the other models, the Dp feature shifted from low values (blue) to high SHAP values (red), indicating that the contribution to MS prediction increases as Dp values increase. This is in accordance with the literature information that increasing the Dp value of a mixture with an average gradation increases the MS [2]. Similarly, in the XGBoost model, bitumen penetration was positively correlated with MS (as bitumen penetration increased, MS prediction increased). The increase in bitumen penetration value provides high performance of the soft bitumen in the mixture at low temperature [30]. Additionally, Gef, Gsb and Dt parameters generally showed a positive effect on MS output. This is consistent with the literature [31-18-32]. In the XGBoost model, CA/FA and Dmax variables showed a decreasing trend with MS. Literature studies show that both an increase in Dmax and an increase in CA/FA ratio may decrease stability [33]. In addition, the variables Wa, Pb, F/B, VMA, Vh and Vf showed both a positive and negative trend in predicting the MS trait. These parameters should be used in optimum proportions as they require some limitations. 2013 Highways Technical Specifications states that volumetric parameters are limited. Also, the F/B ratio should be within a certain range [12-16].

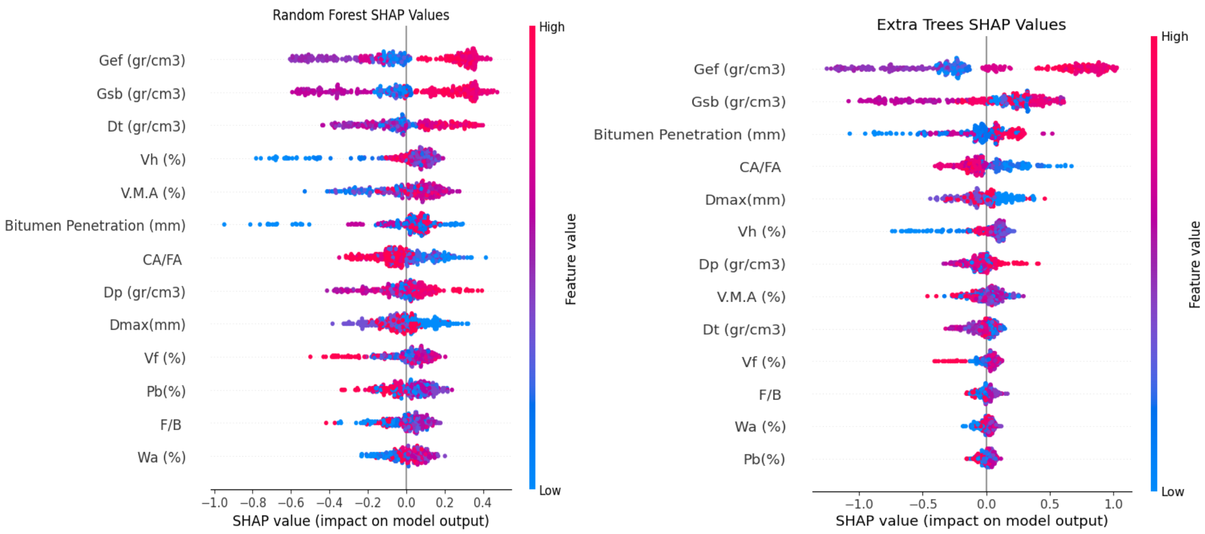


Figure 4. SHAP values for MS value of the models

3.1. Phyton Based Interactive graphical user interface (GUI)

This section is important to describe the development of the XGBoost model, which is the best model obtained using machine learning techniques. A predictive model was designed by optimizing the hyperparameters in the training and testing process of the data collected from laboratory conditions. The GUI model aims to facilitate the preliminary design stages by estimating the MS value as shown in Figure 5. Firstly, the XGBoost model, which was previously trained and saved in pkl file format, was used in the GUI developed for the estimation of the MS value. After entering the data one by one, by pressing the 'Make Prediction' button, the algorithm of the loaded model runs and performs the calculation. The data obtained from Yener's study were tested in the GUI interface. The data were entered separately into the GUI interface. In Table 3, the predicted MS values are compared with the actual MS values [34-35]. As a result, the ratio of the predicted data to the actual data was found to be around 90% on average, which shows the superior generalization capacity of the model.

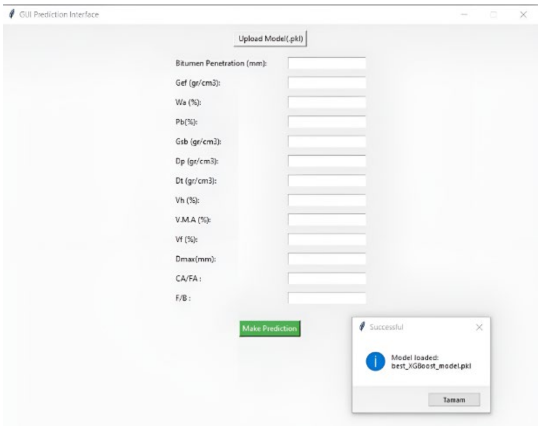


Figure 5. GUI Model

Table 3. Results of Predicting Literature Data

MS Actual (kN)	MS Predicted (kN)	(MS Actual/MS Predicted) (%)
12.59	12.09	104.14
10.39	11.76	88.35
11.37	12.59	90.31
11.17	12.42	89.94
12.03	13.37	89.98
11.74	13.02	90.17
11	12.98	84.75
9.8	13.26	73.91
11.18	10.73	104.19
9.74	10.74	90.69
11.91	11.21	106.24
11.13	10.99	101.27
11.14	10.21	109.11
10.68	10.16	105.12
9.88	10.96	90.15
9.47	10.74	88.18
9.72	12.39	78.45
9.78	11.93	81.98
9.41	11.63	80.91
9.01	11.98	75.21
10.22	10.69	95.60
8.29	10.01	82.82
8.58	10.26	83.63

4. Conclusions

In this study, the MS value in the experimental results obtained from the Van Regional Directorate R&D laboratories in different studies were analyzed. After this data set was preprocessed and organized, data modelling was performed by applying machine learning techniques (Random Forest, GBoost, XGBoost, Extra Trees).

- Among these methods used in predictive models, it was observed that the XGBoost method showed the best performance for predicting the MS value. It was observed that the XGBoost model is a powerful tool for predicting the MS value with high accuracy rates such as 96% R^2 for the test data, low error values (RMSE=0.37%, MAPE=0.02%) and proportional regression performances.

- In this study, SHAP analysis was performed to understand the effect of input parameters on the MS value. The results show that the Gef property has the most positive effect in predicting the MS variable. This emphasizes the importance of consciously adjusting the aggregate and selecting the correct aggregate in quality control tests. In addition, while increasing Dp and Dt increased MS prediction, increasing CA/FA and Dmax generally decreased MS prediction.

- The variables Wa, Pb, F/B, VMA, Vh and Vf have a bidirectional effect on MS, indicating that they require optimum use.

The interface model we developed also provides comparison with different literature data, which is useful in terms of checking the robustness of the model. These evaluations are based on the specific dataset used in the study. The results provide important insights into which parameters should be prioritized in the Marshall design of hot mix asphalt. Moreover, the consistency of the applied machine learning algorithms with the existing literature contributes to facilitating future applications of different Marshall designs and offers preliminary information about the experimental outcomes of asphalt mixtures developed through machine learning. Furthermore, the development of this software algorithm includes errors caused by laboratory test equipment, human factors or material defects. Early detection of such problems enables preventive measures to be implemented, minimizing disruptions to the testing process. Ultimately, this will save both time and cost and significantly improve the overall reliability and efficiency of laboratory operations.

Thanks

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Declaration of Conflict of Interests

The authors declare that there is no conflict of interest. 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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