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OPTIMIZED MACHINE LEARNING METHODS FOR PREDICTION OF MARSHALL STABILITY VALUES

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ABSTRACT

This study evaluates the performance of machine learning algorithms in predicting Marshall stability values to improve quality control processes in highway pavements. Coring is a costly, time-consuming and destructive method, which increases the need for alternative prediction models. In this context, Extra Trees, Random Forest, Gradient Boosting, K-Nearest Neighbours (KNN) and AdaBoost algorithms were used to predict the stability values obtained from core samples and error metrics were analyzed. In the study, the effects of hyperparameter optimization on model performance were examined in detail. The results show that the Extra Trees algorithm has the best prediction performance with an R^2 of 97.62% and an accuracy of 99.71%. Random Forest and Gradient Boosting algorithms also showed improvements after optimization, but their error rates remained higher compared to the Extra Trees model. The KNN model showed moderate success, while the AdaBoost model showed the lowest performance with an R^2 value of 58.87%. The findings reveal that machine learning algorithms can be used effectively in the prediction of stability values obtained from core samples and model performance can be improved by optimizing the right hyperparameters. The study shows that data-driven approaches can be less costly and time efficient in quality control processes.

Keywords: Machine Learning, Marshall Stability, Core Sample, Hyperparameter Optimization

1. INTRODUCTION

In recent years, machine learning (ML) techniques have gained prominence in engineering due to their ability to reduce the cost and time associated with traditional testing methods. In pavement engineering, the destructive and labor-intensive nature of Marshall stability tests has highlighted the need for data-driven alternatives. Supervised ML algorithms, regression models, and hyperparameter optimization have shown promise in accurately predicting stability values from core samples, offering a more efficient and reliable solution.

Although flexible pavements are manufactured to have properties such as flexibility, durability, fatigue resistance, stability and slip resistance, they lose these properties over time due to traffic and climatic conditions [1-4]. In order to evaluate pavements, various tests are performed [5-6], one of the most important of which is coring the pavement, even though it is a destructive method, by extracting the core samples, it can be determined how the aggregate shows physical changes under the compaction processes and traffic load during the construction phase and how the bitumen shows physical changes in the face of production and climatic factors [7-11]. Stability and yield checks can also be performed for core samples [12]. In this way, both material and stability properties of the pavement can be realistically determined. Marshall design method is a widely used method to evaluate the mechanical properties of bituminous mixtures [13-16]. As it is known, one of the most important evaluation criteria of the samples produced for design is stability [17-19]. Stability is also important as a control criterion for core samples taken from the

existing road. However, since the coring process is a destructive method for the road and requires labour and equipment, it is necessary to make predictive approaches on this subject, which is lacking in the literature. Phung, Thanh-Hai Le, Nguyen, Bang Ly, 2023, Marshall stability was predicted using machine learning for asphalt mixtures using basalt fiber. They emphasized that the use of artificial intelligence is promising in engineering problems [20]. Erten and Terzi, 2023, in their study for the reuse of these products by examining the condition of aggregate and bitumen after extraction of core samples taken from existing pavement, they emphasized the importance of asphalt recycling for sustainable transportation [21]. Köfteci, 2017, analyzed the performance of road aggregates that can be obtained from recycling by applying extraction to 20 core samples taken from the bituminous base layer. The author stated that although the aggregates lost some of their properties, they were reusable [8]. Kıyıldı, 2021, whose data are also used in our study, used the Marshall stability values of core samples taken during the construction of Niğde-Adana highway to predict the Marshall stability value with artificial neural networks. In the model with 4 inputs, 15 neurons in the 1st hidden layer, 15 neurons in the 2nd layer and 1 output network structure, it was stated that the prediction made by the ANN was largely consistent with the actual values [12].

2. DATASET AUGMENTATION

In our study, Bitumen as a percentage of the Aggregate by Weight, Bitumen Percentage in the Mixture, Bulk Specific Gravity, Void Percentage in the Mixture values of the core samples given in Kıyıdı, 2021 were used as input data for the developed model [12]. The stability values of the core samples were estimated with the developed models and compared with the estimated values found in Kıyıdı, 2021.

In this study, a data augmentation process was applied to a dataset consisting of continuous variables. Since SMOTE (Synthetic Minority Over-sampling Technique) is only applicable to classification problems, alternative techniques such as Gaussian jittering and sample-based interpolation, which are more suitable for this dataset, were utilized. SMOTE is a method designed for classification problems and cannot be directly applied to regression problems with continuous variables. For this reason, data augmentation techniques such as Gaussian jittering and linear interpolation, which are more suitable for regression problems, are preferred in our study.

The Gaussian jittering method enhances the model's generalization capability by introducing small-scale, normally distributed random noise to existing data points, thereby expanding the dataset. In this approach, minimum and maximum of all variables are determined, and random deviations are added based on a priori defined noise level such that newly generated data points maintain the original distribution. Although Gaussian jittering by itself is not enough to create sufficient diversity, additional techniques such as random sampling and linear interpolation were employed to achieve a more heterogeneous dataset augmentation. Through random sampling, slight modifications were applied to data points selected from the existing dataset, while interpolation was used to generate new points, filling gaps between observed values and promoting a more homogeneous distribution. The combined use of these methods increased the dataset's diversity while preserving its statistical properties, thus mitigating the risk of overfitting and enhancing the model's generalization performance. The results indicate that the augmented dataset largely retains the characteristics of the original data and provides a more stable foundation for training. The pseudocode representation of the data augmentation process is provided in Algorithm 1.

Algorithm 1 Synthetic Data Generation Pseudo Code

```
if additional_samples_needed > 0:
    additional_data = []
    for i in range(additional_samples_needed):
        sample = dataset.random_sample(1)
        jittered_sample = sample.copy()
        for column in dataset.numerical_columns():
            jittered_sample[column] = add_jitter (jittered_sample[column])
        additional_data.append(jittered_sample)
    dataset = dataset.append(additional_data)
save_excel(dataset, "augmented_dataset.xlsx")
```

The 63 rows of data in the existing dataset were increased to 200 rows using augmentation methods. Figure 1 shows the consistency and correlation graphs of the distributions between the original and augmented data set**.**

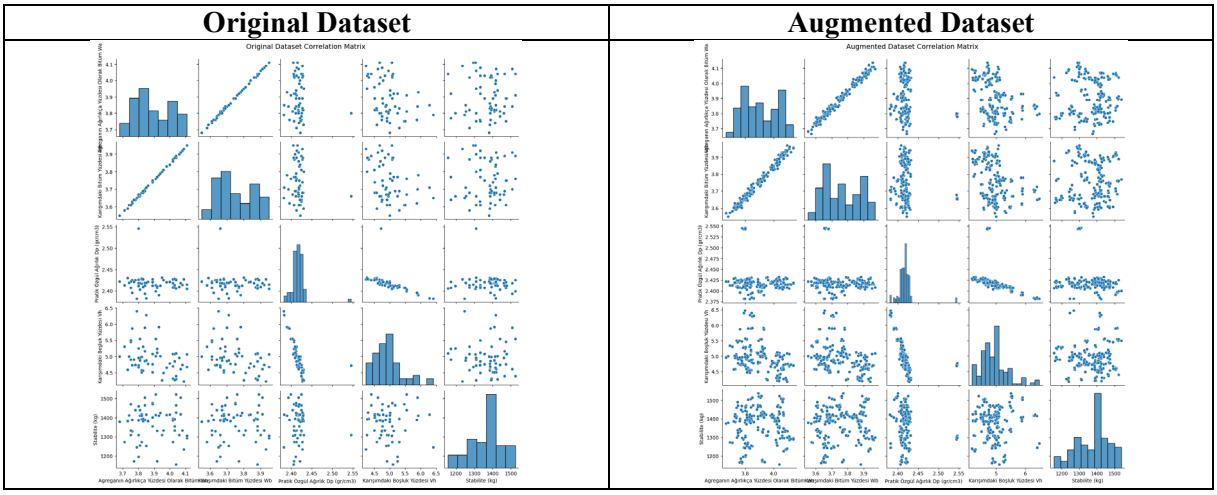


Figure 1. Marshall Core Dataset Augmentation and Correlation Graph

In order to assess the effectiveness of the data augmentation methods, an analysis was performed on the cross-relationship matrices (pair plot) presented above. In the original dataset, it is observed that the distribution between variables has a certain structure. Especially as seen from the histograms, there are intervals where certain variables are concentrated. In the data augmented dataset, the distribution of variables has become denser with the increase in the amount of data. However, it can be said that the overall distribution structure of the data points is quite similar to the original dataset. This shows that the data augmentation process preserved the characteristics of the original dataset to a large extent. Strong linear relationships are observed between certain pairs of variables in the original dataset. In particular, the relationship between "Bitumen W_a as W_t% of Aggregate" and "Bitumen W_b as W_t% of Mixture" shows an almost perfect linear correlation. After data augmentation, this correlation is largely preserved. The data augmentation process was able to expand the data set without disturbing the existing relationships. This shows that the data augmentation method preserves statistical integrity. However, it was observed that the distribution between some variables was widened. In particular, it is observed that the distribution between the "Stability (kg)" variable and other variables has widened. As observed from the histogram graphs, the data augmentation process increased the data density in certain variable ranges. The addition of a small amount of random variation in the data augmentation process has added extra diversity to the data set. However, the general shape of the histograms is largely preserved. The PCA projection shown in Figure 2 shows that the augmented dataset is largely distributed in the same space as the original dataset.

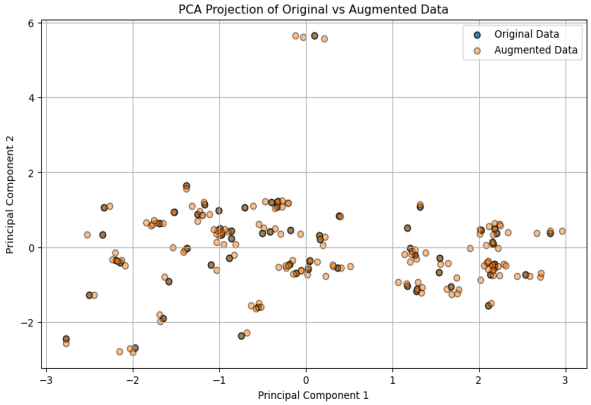


Figure 2. Marshall Core Dataset PCA Analysis

Dark coloured represent the original dataset before augmentation. Light orange points show the new, synthetically generated samples added through data augmentation techniques like Gaussian jittering and interpolation. When the regions where the data points are concentrated are compared, it is seen that the augmented dataset does not disturb the original data structure and preserves the general distribution. This shows that the data augmentation process ensures statistical integrity and extends the dataset without changing its general characteristics. However, the increased density in certain regions indicates that some samples were predominantly derived during the data augmentation process. In particular, new data derived by oversampling or small variations tend to cluster in certain regions. On the basis of principal components, the augmented dataset was found to have the same variance distribution as the original dataset. If the data augmentation process had deviated significantly from the principal components of the original dataset, the newly generated data points would have been collected in a different space. However, the situation observed here shows that the augmented data are appropriately distributed in the original data space and thus the model can reduce the risk of overfitting. In conclusion, the PCA analysis shows that the data augmentation process largely preserves the original data structure but increases the data density in certain regions.

3. ALGORITHMS AND METRICS

In this section, the success, error and prediction values obtained from the machine learning algorithms prepared for prediction will be shown both numerically and graphically. Each algorithm tested for training is analyzed under a separate heading. Each section contains basic and brief information about the algorithm and the results obtained.

The Extra Trees (Extremely Randomized Trees) algorithm is a machine learning method specifically used to solve classification and regression problems. Extra Trees is a method based on decision trees. It uses many trees similar to the Random Forest algorithm as a working logic. In addition, unlike Random Forest, Extra Trees takes more randomness into account when constructing trees [22-23]. G(θ) denotes the prediction function for a single tree, where θ is a random vector defining splits. All trees are combined and averaged into a tree ensemble of G(x), which is generated using the Breiman [22] equation (Equation 1) [24].

$$G(x,\theta_1,\dots,\theta_2)=\frac{1}{2}\sum_{r=1}^{R}G(x,\theta_r) \quad (1)$$

Random Forest builds an ensemble of decision trees using bootstrap samples of the data and selects the best split among a random subset of features. This method improves generalization by decorrelating trees and reduces variance through averaging. The prediction is obtained as Equation 2.

$$\nu=\frac{1}{T}\sum_{m=1}^{M}h_{t(x)} \quad (2)$$

where h_t is the output of each tree.

Gradient Boosting builds models sequentially, each new model trained to minimize the residuals (errors) of the previous ensemble. At each step, a weak learner $h_t(x)$ is fitted to the negative gradient of the loss function, improving overall accuracy. This calculation has made Equation 3.

$$F_{M(x)}=\sum_{m=1}^{M}\lambda_m h_{m(x)} \quad (3)$$

The final model is a weighted sum Equation 4 where λ_m is learning rate.

Error metrics used to determine the success of machine learning models are used to measure the model's performance. These metrics are used to measure the degree of fit of a model's predictions to the actual values and the capacity of the model to generalize. Table 1 shows the comparative results of R2, MSE, RMSE, MAPE, Accuracy, measurements of 5 different machine learning models.

Root means square error (RMSE) was employed in order to compare the prediction errors of different trained models. The closer the RMSE value is to 0, the better the predictive ability of the model in terms of its absolute deviation. The RMSE value is calculated by Equation 4 [24-25].

$$RMSE=\sqrt{\frac{1}{n}\sum_{r=1}^{n}(P_d^{r,m}-P_d^{r,c})^2} \quad (4)$$

The coefficient of determination (R2) is used to estimate model efficiency and is calculated by Equation 5 [24].

$$R^2 = 1 - \frac{\sum_{r=1}^{n}(P_d^{r,m} - P_d^{r,c})^2}{\sum_{r=1}^{n}(P_d^{r,m} - P_d^{-r,m})^2} \quad (5)$$

MSE either assesses the quality of an estimator. The MSE metric is calculated by Equation 6.

$$MSE = \frac{1}{n}\sum_{r=1}^{n}(P_i - P_i')^2 \quad (6)$$

Mean Absolute Percentage Error (MAPE), or Mean Absolute Percentage Error, is a metric that measures the percentage error between predicted and actual values and is calculated by Equation 7.

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{A_i - F_i}{A_i}\right| x100 \quad (7)$$

In the equation n is total number of data points, A_i is the actual values, F_i is the predicted value.

4. FINDINGS AND DISCUSSIONS

Table 1 details the impact of hyperparameter optimization over five different regression models-Extra Trees, Random Forest, Gradient Boosting, K-Nearest Neighbours (KNN) and AdaBoost-on various error and accuracy metrics. After applying hyperparameter optimization, a significant performance improvement is observed in all algorithms.

In the study conducted by Kıyıdı, 2021, it was stated that the relationship between the ANN results and the test results separated for control purposes was $R^2 = 0.91201$.

In this study, Grid Search was employed to optimize the hyperparameters of each machine learning model. For each algorithm, a predefined grid of hyperparameter values was constructed (Table 1), and all possible parameter combinations were evaluated. The optimal configuration was selected based on performance metrics such as R^2 and MSE using cross-validation on the training set.

Table 1. Test results and error metric values of machine learning algorithms

Algorithm & Metric		ExtraTrees	Random Forest	GradientBoosting	KNN	AdaBoost
OPTIMIZED	**R^2**	97.6187	90.4844	90.2832	93.7374	58.8713
	Accuracy	99.7141	98.5282	98.4713	99.0599	96.5564
	MSE	177.135	707.2400	722.1965	466.4547	3063.4103
	MAE	4.0588	20.03795	20.9395	13.2304	48.3017
	MAPE	0.0028	0.01471	0.01528	0.0094	0.03443
	RMSE	13.3092	26.5939	26.8737	21.5975	55.3480
OPTIMIZATION PROCESS	**Parameters and Values for Hyper Parameter Optimization**	n_estimators: [50, 100, 200] max_depth: [None, 10, 20, 30] min_samples_split: [2, 5, 10] min_samples_leaf: [1, 2, 4]	n_estimators : [50,100,200] max_depth: [2, 4, 8, 16] min_samples_split : [2,3,4] min_samples_leaf : [2,3,4,8]	n_estimators : [50, 75, 100] max_depth: [2, 4, 8] min_samples_split : [1,2,4] min_samples_leaf : [1,2 ,8] learning rate : [0.05, 0.1 , 0.5, 1]	n_neighbors: [1, 2, 4, 8] p : [1,2,3,4]	n_estimators : [30, 50, 75, 100,200] learning rate : [0.05, 0.1 , 0.5 , 1, 2]
	Hyper Parameter Values	max_depth: 20 min_samples_leaf: 1 min_samples_split: 2 n_estimators: 200	max_depth: 16 min_samples_leaf: 2 min_samples_split: 2 n_estimators: 50	learning rate: 0.1 max_depth: 4 min_samples_leaf: 8 min_samples_split: 2 n_estimators: 100	n_neighbors: 2 p: 1	learning rate: 2 n_estimators: 100

WITHOUT OPTIMIZATION	**R^2**	97.6170	86.2635	87.2378	80.6169	49.8340
	Accuracy	99.7165	98.2236	98.2823	97.7082	96.3632
	MSE	177.1125	1020.9568	948.5401	1443.7228	3736.5405
	MAE	4.0250	24.0883	23.5265	31.4891	51.3384
	MAPE	0.0028	0.0177	0.01717	0.0229	0.0363
	RMSE	13.3083	31.9524	30.7983	37.9963	61.1272

When evaluating the effects of optimization, R^2 (coefficient of determination) results are one of the most critical measures summarizing model performance. After optimization, the Extra Trees model stood out as the most successful model, offering the highest explanatory power with an R^2 value of 97.61873%. Random Forest, Gradient Boosting and KNN models also showed significant improvements, but the AdaBoost model performed poorly despite optimization. With an R^2 value of 58.87%, AdaBoost did not generalize well to the dataset. This indicates that the model has high variability and inconsistencies in its predictions. In terms of error metrics, Extra Trees was the model with the lowest error rates after optimization. MSE (Mean Squared Error) value was 177.14, RMSE (Root Mean Squared Error) value was 13.31, MAE (Mean Absolute Error) value was 4.0588 and MAPE (Mean Absolute Percentage Error) value was 0.00285. These results show that the Extra Trees model has the lowest prediction error and provides the best fit to the dataset.

Random Forest and Gradient Boosting models also yielded good results by reducing the error values significantly after optimization. Although there is some improvement in the KNN model, error values are greater than other models. The largest error values for the AdaBoost model (MSE = 3063.41, RMSE = 55.34) show that the model cannot generalize well based on the dataset and also contains a very high margin of error. This is a measure of model precision, and the best model is Extra Trees with an accuracy rate of 99.71%. The two best-performing models were the KNN model with an accuracy rate of 99.06% and Random Forest model with an accuracy rate of 98.52%. The worst model was the AdaBoost model at an accuracy rate of 96.55%. The outcome tells us the error rate of the AdaBoost model is higher than other models while its accuracy rate is lower. The low performance of the AdaBoost model may be attributed to its sensitivity to noise and outliers, especially in small and moderately noisy datasets. Since AdaBoost fits regressors sequentially to minimize residuals, early-stage errors may compound, reducing generalization ability.

In summary, as evident, the optimization process influences the performance of the model greatly. Systematic hyperparameter optimization, specifically, has served to decrease the model's error rates, therefore its generalization ability and prediction accuracy. Of the models being considered, Extra Trees was found to be most effective, with Random Forest and Gradient Boosting presenting themselves as good alternatives. The AdaBoost model, however, was not highly successful even with optimization and needs more improvements.

Table 2. Prediction and error scatter plots of all machine learning models

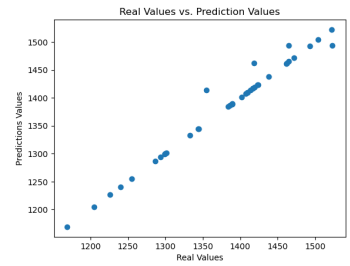
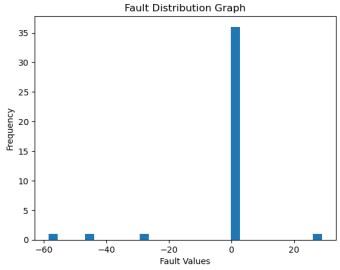
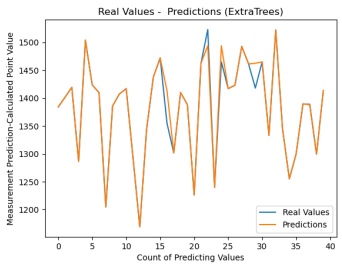
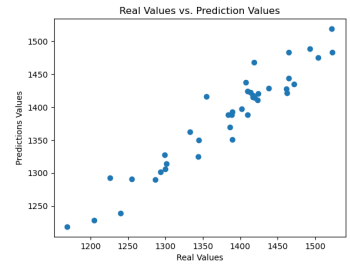
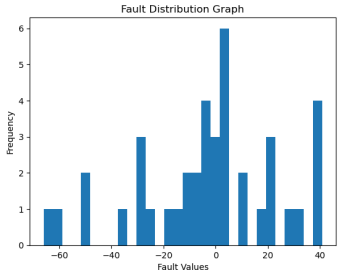
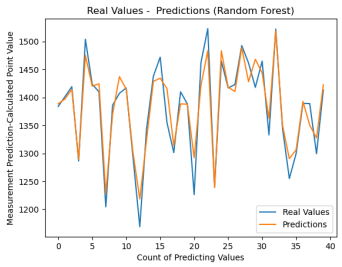
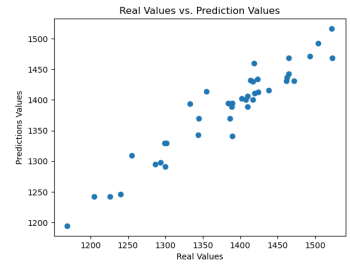
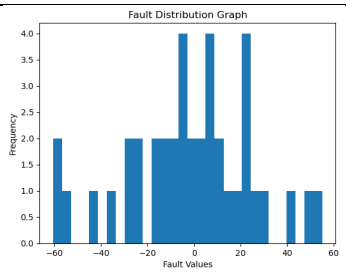
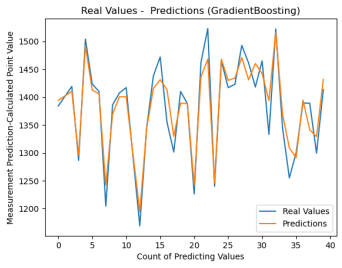
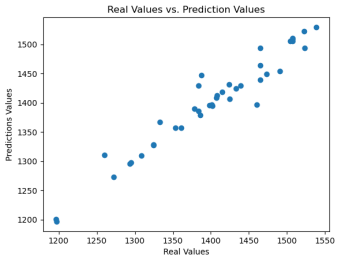
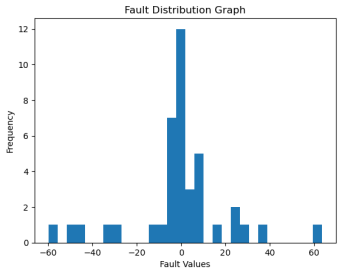
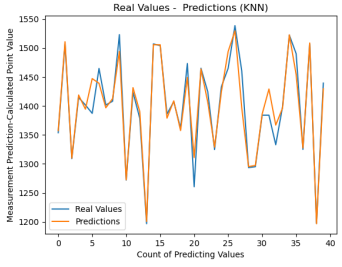
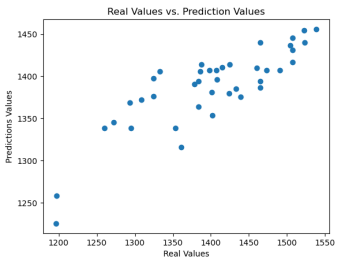
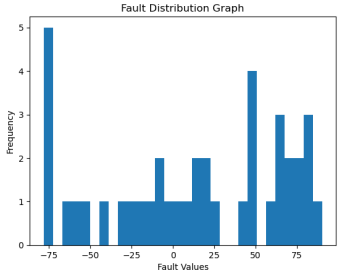
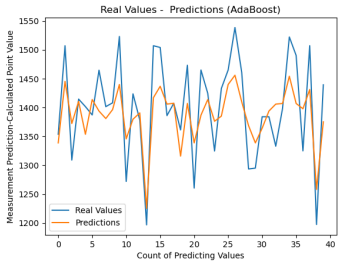
	Model Prediction Graph (Train)	Fault Distribution	Model Prediction Graph (Train &Test)
ExtraTrees			
Random Forest			
GradientBoosting			
KNN			
AdaBoost			

Table 2 provides a comparison of regression performance of five machine learning models (Extra Trees, Random Forest, Gradient Boosting, KNN and AdaBoost) and offers three important analyses per model: Model Prediction Graph - Train, Fault Distribution, and Model Prediction Graph - Train & Test. Training data prediction graphs in the first column investigate whether actual and predicted values are linearly distributed. The Extra Trees, Random Forest and KNN model predictions are more spread towards the actual values, but Gradient Boosting and AdaBoost models are more deviated. This indicates that the first three models better fit the dataset, but Gradient Boosting and AdaBoost deviate more in the

predictions. The plots of error distribution in the second column compare the spread and frequency of errors in each forecast in the models. The Extra Trees and KNN models have minimal deviations in their error distributions, whereas the Random Forest and Gradient Boosting models have a broader error distribution. Surprisingly, the AdaBoost model has the largest variance of errors, indicating that its generalization ability is poorer than the other models. The third column presents the test and training data prediction plot, which is a time series of predicted versus actual values. Extra Trees and KNN models display more stable performance in their predictions compared to the test data, while the prediction errors for Gradient Boosting and AdaBoost models are more pronounced.

5. CONCLUSIONS

In this work, different machine learning models' performances were compared to predict Marshall stability values for quality control on highway pavements. More particularly, Extra Trees, Random Forest, Gradient Boosting, K-Nearest Neighbours (KNN) and AdaBoost algorithms were used to predict the stability values from core samples and their error measurements and accuracy percentages were compared. In the experiment, the before- and after-optimization performance of models is compared and the effect that optimizing hyperparameters have on model performance. From the results, the prediction accuracy of Extra Trees algorithm with R^2 being 97.62% and accuracy rate at 99.71% stands out as the highest. It has the least error measures indicating that the prediction values are quite close to actual values.

The Random Forest and Gradient Boosting algorithms also significantly improved after optimization, but their error rates were worse than the Extra Trees model. The KNN algorithm performed moderately, while the AdaBoost algorithm performed the worst with an R^2 of 58.87% and an accuracy of 96.55%. The increased error rates of AdaBoost suggest that the data set is not likely to be appropriate for this model or that other optimization methods are needed. Additionally, if the graphs of the error distribution are examined, it can be seen that the error distribution of Extra Trees and KNN models are more concentrated, while that of Gradient Boosting and AdaBoost are more dispersed. This study demonstrates that machine learning algorithms can be used effectively to forecast core sample stability values and model performance can be significantly improved by hyperparameter tuning of the appropriate hyperparameters. The findings show how data-driven approaches as an alternative to traditional destructive testing methods can be made cost-effective and time-efficient in quality control processes. Future work will further improve model performance using different feature engineering techniques, deep learning architectures and larger data sets. Additionally, the model's generalization capability will be tested with different core samples of the field to provide a more generalized prediction mechanism for rating the condition of pavement.

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