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Ibrahim Asi * , Yusra Alhadid , Taqwa Alhadidi

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Predicting Marshall Stability and Flow Parameters in Asphalt Pavements Using Explainable Machine-Learning Models

Ibrahim Asi [1], Yusra I. Alhadidi [2] and Taqwa I. Alhadidi [1,*]

[1] Civil Engineering Department, Al-Ahliyya Amman University, 19328, Amman, Jordan
[2] Ph.D. candidate and graduate research assistant, Illinois Center for Transportation; and research fellow, Al-Balqa'a Applied University
* Correspondence: t.alhadidi@ammanu.edu.jo

Abstract: The traditional method for determining the Marshall stability (MS) and Marshall flow (MF) of asphalt pavements is laborious, time consuming, and costly. This study aims to predict these parameters using explainable machine-learning techniques. A comprehensive database comprising 721 hot mix asphalt (HMA) data points was established, including variables such as aggregate percentage, asphalt content, and specific gravity. Models were constructed using the PyCaret Python library, and their performance was assessed using metrics such as the mean absolute error (MAE) and coefficient of determination (R^2). The CatBoost regression model outperformed the other models, achieving R^2 values of 0.835 and 0.845 for MS and MF, respectively. Additionally, Shapley values were used to quantify the variable effects on the predictions. This approach enables the efficient preselection of design variables, reducing the need for extensive laboratory testing and promoting sustainable construction practices.

Keywords: bitumen content; HMA; Marshall flow; Marshall stability; prediction model; SHAP

1. Introduction

The Marshall stability (MS) and Marshall flow (MF) parameters are crucial indicators of the performance and durability of asphalt pavements. Traditionally, determining these parameters requires rigorous laboratory testing, which is not only labor-intensive but also time-consuming and costly. The need for rapid and cost-effective assessment of MS and MF has motivated researchers to explore predictive models that can offer reliable alternatives. Recent advancements in machine- learning techniques present an opportunity to utilize data-driven approaches to predict MS and MF with high accuracy, thereby reducing the dependency on physical testing.

This study focuses on developing explainable machine-learning models to predict the MS and MF parameters of hot mix asphalt (HMA). The objective is to leverage machine-learning techniques to derive robust prediction models that can support the early design phases of pavement construction. Using a comprehensive dataset of 721 HMA data points, the study aims to predict MS and MF using features such as aggregate percentage, asphalt content, specific gravity, and air voids. The explainability of the models is also of prime importance, ensuring that the underlying relationships between variables are understandable by engineers and decision-makers. By providing insights into the contribution of each variable, the study not only aims to predict MS and MF but also to assist in the efficient preselection of design parameters, thereby contributing to more sustainable and economical pavement construction practices.

The machine-learning models developed in this study address key limitations of traditional methods, including the high costs and time requirements associated with laboratory testing. Explainable machine-learning techniques, such as Shapley Additive exPlanations (SHAP), were used to provide transparency into the prediction process, which is critical for gaining the trust of

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engineers and decision-makers. This research aims to offer a practical and efficient tool for predicting asphalt pavement performance, ultimately promoting faster and more reliable infrastructure development.

2. Methodology

The methodology for this study involved several key steps: data collection, preprocessing, model development, and evaluation. A comprehensive database of 721 data points was collected from various sources, representing hot mix asphalt samples with known MS and MF values. The dataset included crucial variables such as aggregate percentage, bitumen content, air voids, specific gravity, and other factors that are known to influence the behavior of asphalt mixtures. These variables were carefully selected based on their relevance to the performance of asphalt pavements.

Data preprocessing was an essential step to ensure the quality and reliability of the models. This step included handling missing values, feature scaling, and splitting the dataset into training and testing sets. Missing values were addressed using appropriate imputation techniques, while feature scaling was applied to standardize the range of the input variables, thus improving the performance of the machine-learning algorithms. The dataset was then split into training and testing subsets, with 80% of the data used for training and 20% reserved for testing the models.

The PyCaret Python library was employed to streamline the model-building process and to compare various machine-learning algorithms efficiently. Several regression algorithms were tested, including linear regression, decision tree regression, random forest regression, CatBoost, and XGBoost. Each model was trained and evaluated using cross-validation to ensure robustness and to prevent overfitting. Model performance was evaluated based on metrics such as mean absolute error (MAE), root mean square error (RMSE), and the coefficient of determination (R^2). These metrics provided a comprehensive understanding of how well each model performed in predicting the MS and MF parameters.

The focus on explainability was a distinguishing feature of this study. Shapley Additive exPlanations (SHAP) values were used to provide insights into how each feature contributed to the model predictions. SHAP values quantify the contribution of each input variable to the prediction, thus enabling a deeper understanding of the relationships between the design variables and the predicted MS and MF values. This level of explainability is crucial for practical applications, as it allows engineers to make informed decisions based on the model outputs.

The overall workflow of the methodology can be summarized as follows:

1. **Data Collection**: Gathering a comprehensive dataset of 721 HMA samples, including relevant features such as aggregate percentage, asphalt content, air voids, and specific gravity.
2. **Data Preprocessing**: Handling missing values, feature scaling, and splitting the data into training and testing sets.
3. **Model Development**: Using the PyCaret library to train multiple regression models, including CatBoost, XGBoost, and others.
4. **Model Evaluation**: Evaluating model performance using MAE, RMSE, and R^2 metrics to identify the best-performing model.
5. **Explainability**: Using SHAP values to interpret the model predictions and understand the influence of each variable.

The CatBoost model emerged as the best-performing algorithm, providing high accuracy in predicting both MS and MF parameters. The SHAP analysis further revealed the importance of key variables such as asphalt content and specific gravity, which were found to have the most significant impact on the predictions. By integrating explainable machine-learning models, this study provides a practical tool for predicting asphalt pavement performance, ultimately supporting the efficient design and construction of durable pavements.

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3. Results

The results of this study highlight the effectiveness of the machine-learning models in predicting the Marshall stability (MS) and Marshall flow (MF) parameters. The CatBoost regression model demonstrated superior performance compared to other models, with an R^2 value of 0.84 for Marshall stability and 0.85 for Marshall flow on the test dataset. The mean absolute error (MAE) for the CatBoost model was 1.25 kN for MS and 0.21 mm for MF, indicating high accuracy in the predictions.

The XGBoost model, while also showing good performance, had a slightly lower R^2 value of 0.81 for MS and 0.82 for MF, with MAE values of 1.45 kN and 0.26 mm, respectively. The linear regression model performed the worst, with R^2 values of 0.63 for MS and 0.67 for MF, suggesting that simpler models may not capture the complex relationships inherent in the dataset.

The SHAP analysis provided valuable insights into the model's decision-making process. Asphalt content was found to be the most influential feature, contributing significantly to the prediction of both MS and MF. Specifically, an increase in asphalt content generally led to an increase in MS and a decrease in MF, indicating a stronger but less flexible mixture. Specific gravity also played a crucial role, with higher specific gravity values being associated with increased stability but reduced flow. The aggregate percentage was another important factor, with finer aggregates contributing to higher stability and lower flow values.

Figure 1 illustrates the SHAP summary plot for the CatBoost model, showing the impact of each feature on the predictions. It is evident that asphalt content, specific gravity, and air voids were the top contributors to the predicted MS and MF values. The SHAP dependence plots further confirmed the nonlinear relationships between these features and the target variables, emphasizing the importance of explainable machine-learning models in understanding complex interactions.

Overall, the results indicate that the CatBoost model can be effectively used to predict MS and MF with a high degree of accuracy. The use of explainable machine-learning techniques ensures that the predictions are not black-box outputs but are instead interpretable and aligned with engineering intuition. This capability is crucial for gaining the trust of practitioners and promoting the adoption of machine-learning models in the field of pavement engineering.

4. Conclusions and Discussion

This study demonstrated the feasibility of using explainable machine-learning models to predict the Marshall stability and flow parameters of asphalt pavements. By leveraging a comprehensive dataset of 721 HMA samples and utilizing advanced regression models, the research successfully reduced the reliance on labor-intensive and costly laboratory tests. The CatBoost model emerged as the most effective model, achieving R^2 values of 0.84 for MS and 0.85 for MF, which indicates a high level of accuracy in capturing the underlying patterns in the data.

The integration of SHAP values to interpret the model predictions provided transparency into the factors that influence MS and MF. The analysis revealed that asphalt content, specific gravity, and air voids were the most influential features, with asphalt content having the greatest impact. This information is valuable for pavement engineers, as it allows for the optimization of mix designs based on data-driven insights. For instance, increasing asphalt content can enhance stability but may reduce flow, which aligns with established engineering principles.

The implications of this study are significant for pavement design and quality control. The ability to accurately predict MS and MF without extensive laboratory testing can facilitate the early optimization of HMA mixtures, saving both time and resources. The use of explainable machine-learning models ensures that the predictions are understandable and can be validated by practitioners, thereby enhancing confidence in the use of these models for practical applications.

Further research could explore the generalizability of the developed models by applying them to other types of asphalt mixtures and conditions. Additionally, future studies could investigate the use of larger datasets and more advanced feature selection techniques to further improve model accuracy. The combination of machine learning and explainability offers a promising pathway for advancing the field of pavement engineering, ultimately leading to more efficient and sustainable construction practices.

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