LYCE NDOLO UMBA

PREDICTION OF HIGH TEMPERATURE PERFORMANCE OF GEOPOLYMER MODIFIED ASPHALT BINDER USING

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Lyce Ndolo UMBA

Supervisors

Assist. Prof. Dr. Gebre Gelete KEBEDE (Supervisor)

Assoc. Prof. Dr. Shaban Ismael ALBRKA (Co- Supervisor)

Nicosia

February, 2025

Approval

We certify that we have read the thesis submitted by Lyce Ndolo Umba titled "**Prediction of high-temperature performance of geopolymer modified asphalt binder using machine learning and model interpretation approach**" and that in our combined opinion it is fully adequate,in scope and in quality, as a thesis for the degree of Master of Master Sciences.

Examining Committee	Name-Surname	Signature
Head of the Committee:	Assist. Prof. Dr. Mustafa Alas	....
Committee Member*:	Assist. Prof. Dr. Ibrahim Sulaiman	....
Supervisor:	Assist. Prof. Dr. Gebre Gelete Kebede	....
Co-Supervisor:	Assoc. Prof. Dr. Shaban Ismael Albrka	....

Approved by the Head of the Department

.09/.04./20.25

Prof. Dr. Kabir. Sadeghi..

Prof. Dr. Kabir Sadeghi

Head of the Department

Approved by the Institute of Graduate Studies

....../...../ 20...

Prof. Dr. Kemal Hüsnü Can Başer

Head of the Institute of Graduate Studies

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I hereby declare that all information, documents, analysis and results in this thesis have been collected and presented according to the academic rules and ethical guidelines of Institute of Graduate Studies, Near East University. I also declare that as required by these rules and conduct, I have fully cited and referenced information and data that are not original to this study.

Lyce Ndolo Umba

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Lyce Ndolo Umba

Abstract

Prediction of High-temperature Performance of Geopolymer Modified Asphalt Binder Using Machine Learning and Model Interpretation Approach

Lyce Ndolo Umba

M.Sc., Department of Civil Engineering

Supervisors: Assist. Prof. Dr. Gebre Gelete Kebede (Supervisor)

Assoc. Prof. Dr. Shaban Ismael Albrka (Co- Supervisor)

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Understanding the rheological properties of asphalt binders is crucial for pavement performance. This research predicts the Storage and Loss modulus, which reflects the elastic and viscous behavior, by applying different machine learning models including XGBoost, Random Forest, and CatBoost. These models were developed using Python. Evaluation techniques like R^2 (coefficient of determination), RMSE (Root Mean Square Error), MAE (Mean Absolute Error), and MAPE (Mean Absolute Percentage Error) were used to assess model predictive performance. Subsequently, model interpretability techniques: SHAP, LIME, ICI, PDP, and PFI to better understand how different features impact the predictions. The results indicated that the CatBoost model achieved significant performance with high R^2 values in training and testing models with lower metrics. Shear stress, temperature, and frequency are ranked as the most important and influential features across all the models for both predictions while softening point, binder type, and viscosity had minor contributions.

Key words: machine learning, storage modulus, loss modulus, models interpretability

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List of Abbreviations

RF:	Random Forest
XGBoost:	Extreme Gradient Boosting
CatBoost:	Categorical Boosting
G':	Storage Modulus
G":	Loss Modulus
PDP:	Partial Dependence Plot
PFI:	Permutation Feature Importance
SHAP:	Shapley Additive Explanation
LIME:	Local Interpretable model agnostic explanations
ICI:	Individual Conditional Importance
R^2:	Coefficient of determination
RMSE:	Root Mean Square Error
MAE:	Mean Absolute Error
MAPE:	Mean Absolute Percentage Error

CHAPTER I
Introduction

1.1 Background

The durability of road infrastructure under traffic loads is highly dependent on the quality of the materials used for its construction; asphalt binders are not an exception in this respect (Lamontagne et al., 2001). Asphalt binders are viscoelastic, meaning that at high temperatures, they cease to be elastic and start to flow viscously. With the rise in temperature, it provides more chance for high-temperature rutting which may cause irreversible pavement deformation due to softening of binder (Zhou et al., 2021). In such scenarios, the development of asphalt binders that would retain mechanical integrity under extreme heat stress is highly required. All these reasons create a demand for durability and sustainability, making it feasible to do the application of geopolymer technology in the asphalt mixtures themselves. It has been determined through research that the modification of geopolymer increases the complex modulus of asphaltic mixtures while reducing their rutting susceptibility, hence exhibiting an increase in its high-temperature stability (Xie et al., 2017) . About high-temperature stability, the modification by geopolymer improves it through raising the complex modulus of asphalt while lowering its susceptibility to rutting (Zhang et al., 2021).

In addition, the modification process will enhance overall durability in severe weather and high traffic, as well as producing high-temperature performance of asphalt mixture. It is hard to predict how the geopolymer-modified asphalt binders can behave in hot conditions because rheological characteristics and performance outcomes are correlated; for that, machine learning algorithms are able to predict how various geopolymer-modified asphalt compositions would behave at high temperatures (Roja et al., 2021). Conventional methods, such as DSR tests, are usually applied for the rheological characterization of asphalt binder; however, these methods generally do not identify the intricate relationships between variables that influence the behavior of the binder.

This has, over the past decade, led to an increase in the application of machine learning methods for predicting the performance in asphalt mixture, thereby allowing for intricate data analyses that give out trends that may be difficult for the classic approaches. Considering geopolymer content, binder properties, and prevailing environmental conditions, the models provide accurate prediction about the behavior that the geopolymer-modified asphalt binders are likely to exhibit at high temperatures (Golestani et al., 2015). These prediction models will enable engineers to determine the best mix designs that meet performance requirements.

1.2 Problem Statement

The high-temperature performance of asphalt binders is of great importance, as it considerably influences the durability and longevity of pavement constructions (Li et al., 2021). The viscoelastic characteristics of asphalt binders are very important because they define how well the material will perform at a wide range of temperatures, high temperatures being a special challenge for pavement longevity (Ali et al., 2017). Traditional methods for the assessment of asphalt binder characteristics are very often costly and time-consuming. This has made it necessary to have an increased need for better methods of prediction, where machine learning methods have great potential. However, machine learning methods also suffer from problems of interpretation, where, for instance, it is usually hard for the researcher to realize how different features influence the final results.

1.3 Aim and Objectives of the Study

This research will, therefore, focus on the incorporation of model interpretability methodologies to explain the variables that affect the predictions of machine learning models. The goal is to improve the performance at high temperature of geopolymer-modified asphalt binders and to develop reliable, data-driven methods to support the creation of more resilient and sustainable pavement designs.

The following are the study's objectives:

- To estimate the storage and loss modulus of the modified asphalt binder using machine learning models, such as Extreme Gradient Boosting (XGBoost) and Random Forest (RF), as well as Categorical Boosting (CatBoost) for high-temperature prediction.

- Feature importance analysis using model interpretation techniques such as Partial Dependence Plot (PDP), Permutation Feature Importance (PFI), Shapley Additive Explanation (SHAP), Local Interpretable model agnostic explanations (LIME), and Individual Conditional Importance (ICI).
- To evaluate the trained model using performance metrics

1.4 Significance of Study

- The significance of this study lies in its capacity to accurately anticipate the behavior of geopolymer-modified asphalt binder at high temperatures, hence improving road durability.
- The environmental effect of road repair and maintenance can be decreased by using geopolymer in asphalt binders. Furthermore, it makes a substantial contribution to material science by expanding the knowledge of the future-useful interactions between asphalt binders and geopolymers.
- Finally, the research shows how particular computer models can be used to solve issues relating to roads.

1.5 Scope of the Study

The present work focuses on the prediction of asphalt binder's performance when treated with geopolymers, especially at high temperatures. Machine learning approaches have been extensively used in a lot of optimization problems, but there is a lack of research when it comes to interpreting the prediction model. This opens new avenues from where outcomes can be compared.

One of the major components used in the development of roads is asphalt binders. Further, its performance has a huge implication on pavement durability and safety. It is possible to apply geopolymers-a type of inorganic polymer-to asphalts for improved characteristics. This research seeks to understand how the modification of the geopolymer affects asphalt binder behavior. To predict these, machine learning methodologies come into play. For the performance of asphalt binders, model interpretations are used by experimental data in correspondence with local and global effects, and local and global interaction measurements.

1.6 Thesis Organization

- Chapter one introduces the topic by giving the problem statement, aims, objectives, and significance of the research
- Chapter two highlights the previous studies related to this research
- Chapter three provides the details on methods used in the study.
- Chapter four discusses the finding result.
- Chapter five concerns conclusion and recommendation for future studies

CHAPTER II

Literature review

2.1 Introduction

The behavior of asphalt binders is a significant factor in the project and application of asphalt since it plays a key role in the durability and service life of this kind of pavement. Elevated melting points can cause greater viscosity, rutting susceptibility, and compromised overall performance of asphalt binders. Many studies have been conducted to improve the high-temperature performance of asphalt binders through modifications and additives related to both rheological properties and resistance to deformation.

Asphalt binders' viscosity is known to be one of the most important factors controlling high-temperature performance. Research has revealed that the use of carbon nanomaterials (e.g., graphene, carbon nanotube) can considerably enhance asphalt binders´ apparent viscosity. This is due to improved interfacial interactions and the restricting molecular chain movement of the binder itself at high-temperature compression, which enhances the flow resistance of the binder under elevated temperatures (Li et al. 2021).

Incorporating polymers specifically of Styrene-Butadiene-Styrene (SBS) into asphalt has extensively been researched. The SBS-modified asphalt not only has higher softening points but also shows less permanent deformation which makes it more suitable for high-stressed applications (Zhang & Hu, 2015). The results of the dynamic shear rheometer (DSR) tests indicate that the anti-rutting factor ($G^*/\sin\delta$) of SBS-modified asphalt increases with an increase in dosage level, indicating improved high-temperature performance, especially at higher temperatures, which have higher $\sin\delta$ index values (Zhang et al., 2019). Although, mixing biochar with other modifiers such as reactive terpolymers has led to the improved rutting resistance and thermal stability of all materials from modified asphalt binder (Dong et al., 2020).

Additionally, waste materials and bio-based additives have turned out to be another significant factor that can provide outstanding performance of the asphalt binders at high temperature. Some of the additives that have been able to provide improvement in the rheological properties of asphalt binders for better resistance against thermal cracking and aging are waste engine oil and biochar (Woszuk et al., 2019). Strong chemical bonds between the geopolymer and aggregate particles help to prevent losses of aggregates and improve the overall cohesion of the asphalt mixture. Improved adhesion has been particularly useful in preventing moisture-related damage occurring in asphalt pavements (Hamid et al., 2020). Therefore, such geopolymers can also be used to enable asphalt binders to have lower temperatures for mixing and compacting. Several advantages come forth during paving with such geopolymers. Not only that, which would serve to add energy conservation, but it would also reduce the emissions related to asphalt production and application when considered on the whole (Katanalp et al., 2024).

2.2 Asphalt in Road Construction

Asphalt plays a vital role in road construction because it is moderately used for pavement as a durable yet flexible and cost-effective material. With increasing pressures for sustainability, some new developments in asphalt technology involve using recycled materials and alternative additives. Incorporation of high recycled asphalt pavement content improves the performance of the asphalt pavements significantly. Toth et al. (2023) underline that full-depth asphalt pavements with high RAP content have not only economic advantages but also positive improvements in in-situ performance, especially for high-volume roads like motorways. This again was confirmed by Sedthayutthaphong et al. (2021) who argued that the addition of reclaimed materials in paving prolongs the service life of pavement on roads, hence the building of environmentally sustainable roads.

This requires adding warm mix additives to reduce the temperature at which the paving is produced, hence reducing the carbon footprint emanating from asphalt production (Toth et al., 2023). One of the most crucial factors affecting the strength and longevity of pavement construction is the bonding between the layers of asphalt, and the mechanical characteristics of asphalt mixtures are among the most significant parameters for the safety and longevity of road surfaces. According to Vaitkus et al. (2011), the effectiveness of each bonding depends upon many factors including aggregate size, binder type, and construction technology

2.3 Asphalt Durability Issues

The performance and life of asphalt pavements is often affected by various durability problems such as fatigue cracking, rut and aging damage caused by moisture.

One of the most common types of distress on asphalt pavements is Fatigue Cracking, which in the most part is generated by repeated traffic loads. These kinds of cracks form when the elasticity of the asphalt binder is broken down by accumulated stress from traffic applications, allowing a crack to develop and may continue to grow with time (Luo et al., 2023). Previous studies considered that fatigue cracking is regarded as one of the main concerns in the design and maintenance of asphalt pavement, and it will affect the structural integrity and the service life of the pavement directly (Hussain et al., 2022).

The other major problem affecting the durability of asphalt is Moisture Damage. Water infiltration into the pavement can lead to loss of adhesion between asphalt binder and aggregates. The result will be the loss of structural integrity of the pavement. This is exacerbated by the phenomenon of rolling traffic over wet surfaces, which generates pore pressure within the asphalt mixture, accelerating deterioration (Sulejmani et al., 2019). As shown by the study of Arfat et al. (2019), moisture sensitivity can be reduced by incorporating some additives that are moisture-resistant in mix design, considering climatic impacts in design. Rutting is a term generally used to describe the permanent deformation of the asphalt surface, which usually develops under high temperatures and heavy traffic loads. The problem is very serious, especially for regions with extremely high temperatures that can cause the softening of the asphalt binder and the layer to deform under the weight of vehicles (Arfat et al., 2019).

The increase in elasticity of the binder, and reduction in temperature susceptibility, among several other areas of improvement, is considered by many previous studies on how to enhance the resistance to rutting. They prove that the polymer modification of asphalt has considerably better properties than unmodified ones (Khasawneh et al., 2023). Crumb rubber can be included as a material in increasing such resistance, which in turn provides rut resistance in improved ways in certain studies (Cheng et al., 2019). Aging is a natural process in asphalts, due to exposure to normal environmental conditions. It leads to hardening of the binder by loss of volatile fractions and becoming brittle. All these degradation mechanisms can lead to increased susceptibility to crack development and overall performance deterioration of flexible pavements (Diab et al., 2019). Some of the innovative systems, like self-healing mechanisms and rejuvenators, have been investigated to neutralize the aging effects, enabling recovery of asphalt properties to a certain extent. Laboratory applications of nanomaterials, such as nano clay, have also been tested for their potential to improve the mechanical properties and durability of asphalt pavements (Iskender, 2016).

2.4 Asphalt Improvement Through Modifications

In particular, research works regarding the performances of asphalt mixes using Styrene-Butadiene-Styrene block copolymers as modifiers abound under high-temperature conditions. Compared with conventional asphalt, SBS-modified asphalt possesses an exceptionally good softening point and much higher resistance to rutting because of high viscosity. Further, besides granting pronounced improvement in temperature stability to asphalt binders, applications of SBS have improved performances for a series of environmental parameters (Li et al., 2023).

This becomes crucial for those pavements that are prone to high temperatures and large volumes of traffic flow as the chances of deformation accordingly become very high. The use of asphalt rubber mixes has also enhanced high-temperature stability for asphalt mixtures apart from polymer modification. Cheng et al. (2019) conducted different types of stress creep recovery tests; the results showed that the incorporation of crumb rubber significantly improves the high-temperature performance of the asphalt mixture and binder. They found that asphalt rubber blends are suitable for high-traffic roads due to their enhancement in pavement durability and rutting resistance. WMA is also regarded as a new approach in the improvement of asphalt mixture performance at high temperatures. It allows lower temperature for mixing and compacting, which is able to enhance workability and simultaneously reduce energy consumption. WMA's lower temperatures of production than HMA can result in an improved quality of binders, together with reduced fumes during construction, hence an environmentally friendly procedure.

Sun et al. (2019) present research that WMA performs just like HMA, especially in terms of high-temperature stability. The addition of diatomite does not significantly affect the low-temperature performance of asphalt mixtures but has proved its potential as an asphalt modifier by enhancing stability at high temperatures. This is a unique property that makes this type of material highly useful for situations where a high level of heat resistance is needed.

Cheng et al. (2019) reported that an increase in the diatomite content of the mixture significantly enhances its rutting resistance. Anti-rutting chemicals have also been tried in modifying asphalt for improved performance at high temperatures. Among them, Liu & Tang. (2023) assert that anti-rutting chemical additives like NRP increase resistance when treated on asphalt mixtures against water and high temperature. Experiments with NRP-modified agents showed that there was a significant reduction in rutting for high-traffic areas, prolonging pavement life in areas that usually have this problem due to high traffic and temperatures. At high temperatures, Sasobit has also been found to act as a warm-mix additive that enhances the rheological characteristics of asphalt binders (Turbay et al., 2022). However, the extent to which Sasobit decreases viscosity depends on the specific formulations and conditions involved (Jamshidi et al., 2012).

2.5 Benefit of Using Geopolymer Modified in Asphalt Mixture

Value-added geopolymers are manufactured from various industrial byproducts, like fly ash, considerably improving both mechanical properties and economic efficiency of asphalt mixes. Given its superior benefits, it has turned out to be an important tool and is now intensively applied in recent modern pavement engineering. In fact, the incorporation of geopolymers in asphalt will modify mechanical properties, above all increasing its resistance to rutting and on the whole boosting durability Hamid et al. (2020). Adding geopolymers to asphalt binders increases their viscosity, thus increasing their resistance to long-term deformation under high traffic. This is because the particle network of an asphalt-geopolymer blend expands for a more stable and effective mixture.

In fact, further research by Bujang et al. (2023) mentioned that asphalt mixtures containing fly ash geopolymers had increased fatigue and rutting resistance, prolonging its service life and reducing maintenance costs, especially under heavy traffic conditions where the performance of the pavement is crucially needed. The rheological properties of asphalt binders treated with geopolymers are also significantly improved; this, in turn, means that geopolymers increase the softening point and decrease the penetration, which is critical to achieving high-temperature performance. Asphalt pavements are prone to thermal deformation and cracking under extreme fluctuations in temperature. In this regard, geopolymers are added to asphalt mixtures between 6% and 9%, according to research for optimal performance (Dulaimi et al., 2023; Bujang et al., 2023). Geopolymers improve adhesion between aggregate particles and asphalt binders for durability.

This is because a recent study by Bujang et al. (2023) shows that the pavement's lifespan is extended due to the fact that the chemical bonding afforded by geopolymers prevents aggregate particles from being lost. As a matter of fact, it is this improved bonding that is needed to maintain the structural integrity of asphalt pavements, considering extreme weather conditions and traffic congestion. The compaction behavior of asphalt mixes reinforced with geopolymers was studied using a sophisticated approach, such as that of DEM. A new modeling approach, in the work by Olsson et al. (2019), was done to shed light on the mechanical interactions occurring within these mixes. This is one of the approaches aimed at aiding engineers in their compaction to achieve particular density and performance objectives. These geopolymer-modified mixes have been tested in various field and laboratory tests. For example, Bujang et al. (2022) conducted volumetric tests of asphalt mixtures containing fly ash geopolymers and observed better performance and stability of the geopolymers as compared to conventional asphalt mixtures.

2.6 The Elastic and Viscous Behavior of Asphalt Binders

The forecast of storage and loss modulus present in asphalt performance helps to explain the viscoelastic behavior of the asphalt binder. While loss modulus defines the viscous behavior of the asphalt material, the elasticity of the material is given by its storage modulus. Their prediction may help engineers understand the resistance that a material can have to deformation for different loading conditions, which becomes an essential part of pavement design (Wang et al., 2020). A material's modulus denotes its stiffness and recovery capacity, the energy retained after deformation due to stress. To avoid permanent deformation under traffic loads, elastic characteristics will be better for larger values of G′ (Wu et al., 2021). The storage modulus of asphalt mixture may be affected by its composition, loading frequency, and temperature. The addition of polymer modifiers like SBS has been proven to raise the storage modulus of asphalt binders significantly and enhances their ability in high temperature storage (Li et al., 2023). On the other hand, a master curve of dynamic modulus can relate G′ with temperature and frequency, for instance by the use of TTSP (Zhang et al., 2020).

A higher loss modulus means that asphalt will be able to absorb more energy from the traffic load. This is important in preventing fatigue cracking, among other forms of distress. Often, the relationship of G′ to G″ is defined by a phase angle δ, where with decreasing phase angle, the behavior is more elastic, while at higher phase angle values, the response becomes more viscous (Bennert et al., 2023). The aging of asphalt can also reduce the loss modulus, where with the hardening of binder, aged binders normally have greater G″ values.

The storage and loss modulus for both have been developed to facilitate design and analysis in asphalt mixtures. Most of these models' basic concepts rely on the experimental data acquired from DSR and subsequently derive G*, which is the complex modulus consisting of both G′ and G″ (Zhan, 2013). Semi-empirical models to machine learning approaches have been made to find a prediction for dynamic modulus from the viscoelastic properties of asphalt mortar and mixtures (Dao et al., 2020). For example, the Hirsch model and Witczak's model are normally applied to estimate the dynamic modulus from material properties and loading conditions (Wang et al., 2021)

2.7 The Use of Machine Learning for Predicting the Performance of Asphalt Mixtures

A new field of study, therefore, is in development to better the precision and effectiveness of the performance evaluations through sophisticated computational techniques for the estimation of the storage and loss modulus of asphalt mixtures by machine learning models. These models require input parameters of temperature, stress conditions, and material composition to forecast the viscoelastic characteristics of asphalt for pavement design and performance assessment. Several of the most popular machine learning techniques for estimating of the dynamic modulus and further the separate parts of its storage and loss modulus of the asphalt mix include Artificial Neural Networks, Support Vector Machines-SVM, and the Random Forest-RF algorithm, widely applied in modeling the mechanistic properties in asphalts (Wang et al. (2021) Dao et al. 2020; Ayazi et al., 2024).

These methods make more accurate predictions than traditional empirical methods and allow for the extraction of complex patterns linked with input variables regarding the intended outcome. Quantitatively and qualitatively, the amount of data utilized for training a machine learning model is major influencing factors on the performance. Dao et al. (2020) are some of the few who have developed predictive models for the dynamic modulus of warm mix asphalt using large laboratory test datasets. In the same way, such comprehensive datasets should be considered to predict the modified reclaimed asphalt pavement mechanical behavior as precise as possible. Also, more complex input features, such as aggregate gradation, binder concentration, and environmental conditions, enhance the performance of the models (Ayazi et al., 2024).

This can be done by using the mean squared error, R-squared values of the machine learning model performance, among other metrics, as some guidelines to assess predictive accuracy. Many literatures have established that hybrid models tend to give better results since they are combined with several machine-learning techniques. For example, Eleyedath & Swamy. (2022) work on a hybrid model for the prediction of the dynamic modulus of asphalt concretes by incorporating the principal component analysis into gene expression programming.

Le et al. (2020) presented a hybrid artificial intelligence model for predicting the dynamic modulus of stone mastic asphalt by combining various algorithms that would provide optimum performance prediction of the materials. This hence underlines the possibility of using multiple machine learning techniques to enhance predictive capability on asphalt mixes. Furthermore, machine learning applications also extend to the assessment of RAP properties. (Botella et al. (2022) applied ML techniques to estimate the degree of binder activity in RAP (reclaimed asphalt pavement) and demonstrated that machine learning can sort out relatively simple input variables and provide very accurate predictions of the performance of recycled materials. This, especially for sustainable construction, will be a more important factor in the future, as more stress is being placed on the use of recyclable materials. Machine learning integrated into asphalt mixture performance prediction enhances the predictive accuracy and contributes to efficiency in the general design process. According to Uwanuakwa et al. (2020), machine learning models are thus applicable for accelerating the tests of various performance parameters, such as rutting and fatigue cracking, which enable the making of informed decisions in asphalt mix design.

This capability is sorely needed to meet challenges in traffic loads and environmental condition uncertainties that have been directly affecting pavement. Model interpretability has become of great significance when it comes to machine learning, especially within critical domains such as healthcare. Different explanation methods have cropped up, like SHAP, LIME, PDP, ICI, and PFI which let model transparency go hand in glove with trust. According to (Swathi & Challa, 2023), techniques could be divided into two important interpretability approaches, global and local, each reflecting a different insight upon model behavior. Global methods aim to provide insights on the whole conditional distribution, while local ones give insight for certain instances (Molnar et al., 2022). Research is done concerning their power of explanation and identifying relevant or important features (Tiwari et al., 2019).

CHAPTER III

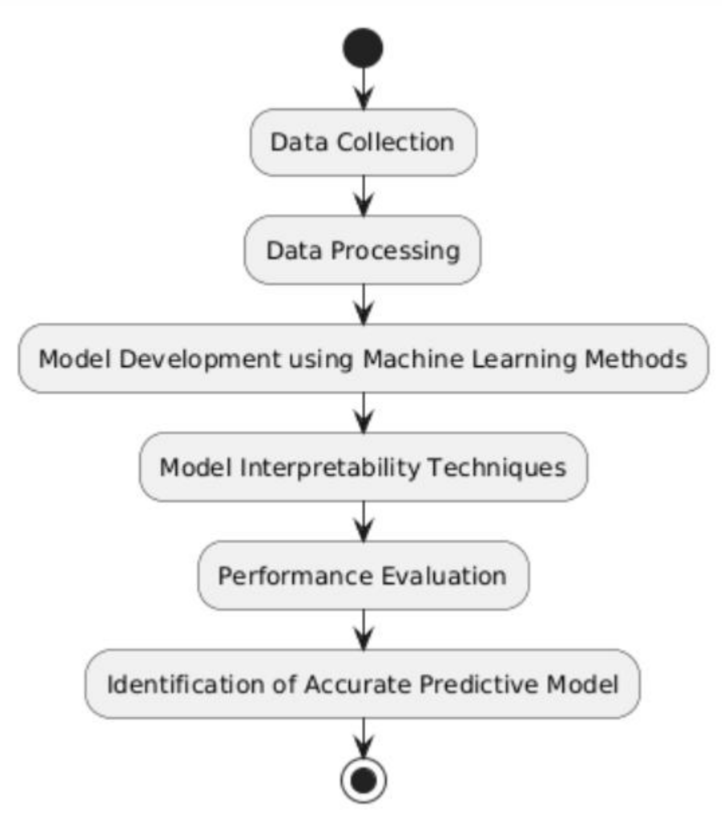
Methodology

3.1. Proposed Methodology

This research proposed tree machine learning models including Random Forest (RF), Extreme Gradient Boosting (XGboost) and Categorical Boosting (CatBoost) to predict the high-temperature performance of geopolymer-modified asphalt binder using local and global effect and interaction analysis. A proposed schematic diagram for methodology is presented in Fig 1 which, includes stages of data collection, data processing, model development using machine learning methods, model interpretability techniques, performance evaluation, and identification of the accurate predictive model.

Figure 1

Proposed schematic diagram for methodology



3.2. Data Source and Processing

The data used in the research was obtained from physical tests: penetration, softening point, viscosity, conducted according to ASTM D5, ASTM D36, and a rheological test using a dynamic shear rheometer (Frequency sweeps tests) according to AASHTO T315 (Ali et al., 2017). The 60/70 penetration grade was the base asphalt, whereas the geopolymer modifier of asphalt binders was a mixture of Fly Ash and alkali liquid which was a sodium silicate solution Na2SiO3 and sodium hydroxide NaOH pallet diluted in water to produce an 8 Molar (8M) of NaOH solution, while the Class F fly ash had a Specific Gravity -2.26. The mixture of Na2SiO3 and NaOH was prepared to activate the alumino-silicate precursors in fly ash through a series of dissolution-hydrolysis. Nine (9) explanatory parameters have been used for this study which is composed of seven (7) inputs and two (2) outputs, represented in the following table:

Table 1.

Features distribution of dataset

Name	Measurement	Data type	Description
Type of binder	Percentage	Qualitative	Input parameter
Temperature	Celsius	Quantitative	Input parameter
Frequency	Hertz	Quantitative	Input parameter
Shear stress	Pascal	Quantitative	Input parameter
Softening point	Celsius	Quantitative	Input parameter
Viscosity	Pascal	Quantitative	Input parameter
Failure temperature	Celsius	Quantitative	Input parameter
Storage modulus	Pascal	Quantitative	Output parameter
Loss modulus	Pascal	Quantitative	Output parameter

Table 2.

Descriptive statistics

	Type of Binder	T in °C	Frequency (f) in Hz	Shear stress (τ) in Pa	Softening point (°C)	viscosity @135	Failure temperature	Storage modulus (G') in Pa	loss modulus (G") in Pa
Mean	3.345	62.646	4.204	4865.538	51.161	0.410	66.169	1374.178	8499.403
Standard Error	0.164	0.789	0.345	445.162	0.255	0.003	0.3164333	344.739	1332.599
Median	3	64	1.592	2142.550	49	0.41	67	75.729	1775.103
Mode	0	46	15.92	1228.04	47	0.35	59	35.277	1028.365
Standard Deviation	2.474	11.862	5.182	6692.258	3.841	0.042	4.757	5182.574	20033.355
Sample Variance	6.120	140.719	26.848	44786323	14.755	0.002	22.629	26859074	401335333
Kurtosis	-1.223	-1.171	0.377	6.592	-1.528	-1.281	-1.207	66.649	34.295
Skewness	-0.105	0.174	1.316	2.423	0.361	-0.345	-0.650	7.486	5.177
Minimum	0	46	0.1592	12.913	47	0.35	59	0.537	10.829
Maximum	7	82	15.92	32626	56.5	0.46	71	56366.602	183713
Count	226	226	226	226	226	226	226	226	226

To obtain good performance, the data must first be pre-processed before being evaluated by machine learning algorithms. Data normalization is a pre-processing technique that involves scaling or transforming the data so that each feature contributes equally (Dalwinder Singh & Birmohan Singh, 2020). By using this pre-processing step, all features were appropriately scaled to fall between 0 and 1. The min-max normalization was used using the equation below:

$$X_i' = \frac{X_i - X_{min}}{X_{max} - X_{min}} \quad (1)$$

where,

X_i is the observed data while, X_{max} *and* X_{min} represent the maximum and minimum value of the data.

3.3. Machine Learning Models

3.3.1. Random Forest (RF)

Random Forest is mainly an ensemble learning method that has widely been used both for classification and regression problems in machine learning (Ren et al., 2016). After training, this algorithm creates multiple decision trees and gives the mode of classes in the case of classification, or the mean prediction among different trees in the case of regression, as output, as was proposed (BREIMAN, 2001). It works quite effectively on big and high-dimensional data sets, with applications ranging across diverse domains.

Random Forests are based on bagging (bootstrap aggregating) algorithm combined with decision trees. That is, multi-numbers of decision trees trained on various subsets of the training data. Each is built by a random sample of points in data and a random subset of features. This decorates the trees from each other. The diversity among the trees would decrease the risk of overfitting; in contrast, single-decision trees do have this problem. The final prediction is obtained by aggregating the predictions from all these trees, enhancing their overall accuracy and robustness within the model (Zhang et al., 2021)Li et al., 2020).

Compared to single decision trees, the main advantage of the Random Forest model is that it has less risk of overfitting, especially when there is noisy data. The major impacts of averaging multiple trees include smoothing predictions and a reduction in variance (Elmuna et al., 2023). It can handle missing values effectively because it keeps accuracy steady even when a large portion of the data is missing since its prediction depends on the majority of the trees based on available data. Further, an additional advantage of Random Forests is that it provides insight into feature importance. The features would be ranked according to their contribution to the prediction, and this may turn out to be informative in the understanding of the underlying data, and it could also serve in the selection of features (Y. Liu et al., 2018). It is an extremely friendly algorithm to practitioners, mainly because it requires minimal pre-processing of the data. The data does not necessarily be scaled or normalized, therefore making life so easy for the modeling process. According to (Xu et al., 2012) Random Forest can handle imbalanced datasets much better compared to many other algorithms; this is because its tuning can be done to focus on minority classes without losing overall accuracy (Zhang et al., 2020).

3.3.2. Extreme Gradient Boosting (XGBoost)

XGBoost, or Extreme Gradient Boosting, is a popular ensemble learning algorithm that falls under the family of gradient boosting methods. Generally, it is put to work in supervised learning tasks much like random forests for classification and regression problems. However, it is known for its speed and efficiency in the execution of big data and complex models (Chen & Guestrin, 2016). It is based on the boosting ensemble technique, which pools predictions from a set of weak learners simple decision trees to come up with a strong predictive model (Lv et al., 2021). In a boosting model, XGBoost votes to build trees in order, with each new tree trying to correct the errors made by previously grown trees. It does this by optimizing a loss function using gradient descent in a way that iteratively minimizes the prediction error (Bi et al., 2020). The structure of XGBoost consists of several components:

- Decision Trees: XGBoost constructs an ensemble of decision trees where each tree is built based on previous residual errors. The trees will be added sequentially, one by one, with each contributing to the final prediction (Yang et al., 2024).
- Learning rate: The learning rate or shrinkage parameter defines the contribution of each tree to the final prediction. For a given lower learning rate, increasing the number of trees improves the model for performance at the cost of slow training.
- Objective Function: is a combination of a loss function, which calculates the difference between predictions and actual values, and a regularization term. The latter punishes model complexity for better generalization. This can be formally expressed as:

$$Obj^{(t)} = \sum_{i=1}^{n} l\left(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)\right) + \Omega(f_t) + constant \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Where l is the loss function, n is the sample size, y_i is the observed values, $\hat{y}_i^{(t-1)}$ is the predicted value of the last iteration, f_t is a new function which model learns, x_i is the feature vector and $\Omega(f_t)$ denotes the regularization term which saves the model from complexity.

- Hyperparameters: Among the hyperparameters that can be optimized in XGBoost are the number of trees, the maximum tree depth, the subsample ratio, and the regularization parameters (Torlay et al., 2017).

The number of trees, maximum tree depth, subsample ratio, and regularization parameters are examples of hyperparameters that need to be tuned carefully for the best performance to be achieved from XGBoost (Torlay et al., 2017). Indeed, in most practical applications, this model outperforms a large number of other machine learning methods due to its well-known high predicted accuracy and efficiency (Bi et al., 2020). It is one of the favorites of data practitioners due to its capability to handle big datasets with complicated interactions. XGBoost accepts a wide range of input formats and problem domains such as regression, multiclass classification, and binary classification (Liu et al., 2022). It is also resistant to overfitting because of its sophisticated regularization methods, hence suitable for noisy and high-dimensional data (Romeo & Frontoni, 2022). It also helps in feature selection and model interpretation by providing useful information on which features have a major impact on model predictions through the feature significance method in XGBoost (Yang et al., 2024).

3.3.3. Categorical Boosting (CatBoost)

The gradient-boosting technique CatBoost makes use of binary decision trees. It improves on conventional gradient boosting by resolving problems such as overfitting and bias (Dorogush et al., 2018). This is how it functions:

- Sequential Training: CatBoost trains on the entire dataset sequentially to reduce bias.
- Random Permutation: After training, the dataset is randomly permuted.
- Average Label Calculation: For each sample, an average label is computed based on the permuted data to prevent overfitting.

CatBoost effectively transforms categorical features into numerical ones by utilising an ordered boosting technique created by Prokhorenkova et al. (2018). It overcomes the problem of gradient bias in the traditional gradient-boosting decision tree by ensuring that the conversion retains as much information as possible and hence minimizes information loss and overfitting caused by biased gradient estimates. Ordered Boosting is explained as follows:

Ordered boosting algorithm

Input: $\{(X_k, Y_k)\}_{k=1}^{n}, the\ number\ of\ trees\ I$;

$\sigma \leftarrow random\ permutation\ of\ [1, n]$;

$M_i \leftarrow 0\ for\ i = 1, \ldots\ldots, n$;

$for\ \ t\ \leftarrow 1\ to\ I\ do$

$for\ \ i\ \leftarrow 1\ to\ n\ do$

$r_i \leftarrow y_i - M_{\sigma(i)-1}(X_i)$;

$for\ \ i\ \leftarrow 1\ to\ n\ do$

$\Delta M \leftarrow LearnModel\big[\big(X_i, r_j\big): \sigma(j)\ \le i\big]$;

$M_i \leftarrow M_i + \Delta M$;

$return\ M_n$

This algorithm is according to σ, which is an example of a random permutation of data, $\{(X_k, Y_k)\}_{k=1}^{n}$ representing a dataset with X_k as the input feature and Y_k as the target variable for each sample k. The data indices $[1, n]$ are randomly permuted to produce a new order of samples. For t = 1 to I, the model prediction (M_i) is initially equal to zero, but it will be updated as I trees are sequentially added. The residual (r_i) of the I sample is computed as the difference between y_i the actual target and $M_{\sigma(i)-1}(X_i)$ the current model prediction, then the weak model learner's contribution ΔM is added to the model prediction for all samples to updated it. Finally, the algorithm returns the ensemble model (M_n) after I interactions.

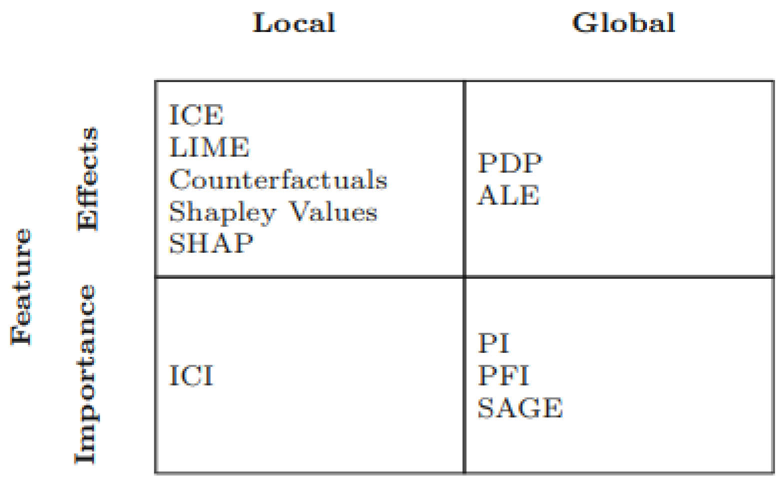
3.4 Model Interpretation

Model interpretation is one of the various methods used to make sense of the way a machine learning model is making predictions (Poursabzi-Sangdeh et al., 2021). ML has greatly improved and shown applications in many areas. This element is very crucial for high-stakes situations where transparency has to be (Miller, 2018). Improving Machine Learning Model Interpretability addresses both educational goals and interest in how algorithms derive predictions. Moreover, explainability enhances the security of these models through testing, evaluation, and improvements. This is most important in sectors where mistakes have high impacts, such as fatal ones. Interpretable machine learning can be achieved using various techniques that have unique qualities.

According to Molnar et al. (2022), the above two approaches have traditionally been divided based on the feature effects and feature importance of either a single data point or entire dataset - respectively: in Figure 1; this has two interpretations, which are explained in terms of Global Interpretability and local interpretability, whereas, during Global model interpretability: aims at insight into how specific features contribute toward predictions, overall on any data set. Partial Dependence Plots and Accumulated Local Effects are two methods that will give an overall view of how each feature affects the model's predictions across all data points. Global Importance Approaches such as Partial Importance, Permutation Feature Importance, and SAGE are used to quantify each feature's contribution to the model's prediction ability. With these methods, the contribution or influence of every feature towards the model's overall performance is assessed.

Figure 2.

Techniques for Understanding Machine Learning Models (Molnar et al., 2022).



		Local	Global
Feature	Effects	ICE LIME Counterfactuals Shapley Values SHAP	PDP ALE
	Importance	ICI	PI PFI SAGE

The main goal of local model interpretability is individual prediction explanation. Local importance presents the degree a feature that affects a particular prediction using Individual Conditional Importance (ICI). The contribution of each feature to a particular prediction is quantified with techniques such as Shapley Additive Explanation (SHAP), Individual Conditional Expectation (ICE) curves, and Local Interpretable Model-agnostic Explanations (LIME) to understand the local effects on predictions. This study applied SHAP and LIME to assess the local impact on predictions, Individual Conditional Importance (ICI) for the evaluation of local importance, Partial Dependence Plots (PDP) for understanding the global general effect of features, and Permutation Feature Importance (PFP) to determine the global feature importance.

3.4.1. Local Interpretable Model Agnostic Explanations (LIME)

LIME is the method that explains the predictions of complex machine learning models in a more understandable form. It creates a much simpler and understandable model that emulates the behavior of the original "black-box" model for a certain given neighborhood of the given instance. This locally produced approximation, though with important overviews into the inner working mechanisms for normally incomprehensible models, gives insight into the decision-making process.

The central idea behind LIME is to perturb the input data and study how changes in the data affect the output of the model (Dindorf et al., 2020 ; Sousa et al., 2019). It does this by creating a set of altered samples surrounding the instance to be explained, after which a simple local model-fitting, such as a decision tree or linear regression, is fitted to closely mimic the behavior of the original model within that region. This procedure enhances our understanding of the internal model logic by elucidating how certain predictions are made and showing which characteristics have the most value for a specific choice (Dindorf et al., 2020).

3.4.2. Shapley Additive Explanation (SHAP)

SHAP is a well-known Approach for ML model analysis using Cooperative game theory with the explanation by Shapley values, and is developed by Lundberg & Lee., (2017). This calculates the contribution of each feature towards the outputs from the model's prediction. According to Rodríguez-Pérez & Bajorath. (2020) in a unified approach, SHAP examines features reliance on consequences of even sophisticated, complex models of any design.

The most important advantage of SHAP is its additive property, which states that the difference between the model's prediction for an individual instance and the average prediction across all instances is equal to the sum of SHAP values for all features. This property greatly enhances the interpretability and transparency of the explanations, while providing a uniform approach to estimating the contribution of each factor (Wang et al., 2022).

3.4.3. Individual Conditional Importance (ICI)

The particular strategy for the discovery of the most influential variables locally will be called the individual conditional importance. That enables learning about how a specific model's feature produces a specific forecast. ICI thus gives insight into a better investigation of different feature relevance in different portions of data and introduces the application of the concept of Shapley values. It reinforces the confidence level and understanding with a critical sense of trust in the way decisions are done via models, by describing how various subsets influence the prediction (Casalicchio et al., 2019).

3.4.4. Partial Dependence Plot (PDP)

Partial Dependence Plots (PDPs) show the relationship between a machine learning model's prediction and one or more input features. They are particularly helpful for analyzing complex models because it can be difficult to determine how a specific attribute affects the results just by looking at the model's structure. PDPs are the most straightforward methods for communicating the relationships between these features and the target variable because they represent the marginal impact of a single feature on the expected outcome, averaged over the other features (Friedman, 2001).

3.4.5. Permutation Feature Importance (PFI)

The significance of features in machine learning models is frequently assessed using Permutation Feature Importance (PFI). The methods measure the accuracy decrease that happens when feature values are randomly shuffled to quantify the distribution of features on the performance model.

This is particularly a very useful method in that it is model-agnostic; it can be applied to any trained model, irrespective of its underlying architecture. The PFI quantifies features' importance by measuring how far the model's accuracy is influenced when the feature values have been permuted, in most PI, attention has turned to the marginal impacts while adjusting for the impact brought forward by other variables (Brenning, 2023).

3.5 Model Evaluation Methods

In this research, various methods are used to quantify the error and variance in a forecasted dataset, with no particular technique being better than the others (Muliauwan et al., 2020). The techniques employed include mean absolute error (MAE), root mean squared error (RMSE), mean absolute percentage error (MAPE), and R-squared as error evaluation metrics that can be mathematically expressed by:

$$R^2 = 1 - \left(\frac{\sum_{i=1}^{n}(y-y')^2}{\sum_{i=1}^{n}(y')^2}\right) \tag{2}$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y - y')^2} \tag{3}$$

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{y-y'}{y}\right| \tag{4}$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y - y'| \tag{5}$$

where the number of data is n, and the actual and anticipated values are y and y' respectively. RMSE measures the average discrepancy between each real data point and the anticipated outcomes. Using the absolute difference between the actual data and the anticipated outcomes, MAE computes the average error. R quantifies the degree of the linear relationship between the two variables. While it shares similarities with MAE, which computes absolute differences in accuracy. The benefit of MAPE is that it is more effective at identifying the relative differences across models because it is unaffected by the unit or magnitude of the anticipated and actual values

CHAPTER IV
Results and Findings

4.1 Introduction

In this section, the research presents all machine learning models mentioned in chapter three, including Random Forest (RF), Extreme Gradient Boosting (XGBoost), and Categorical Boosting (CatBoost). They were utilized to predict the storage modulus (G'), and loss modulus (G") of geopolymer-modified asphalt binder. The results of all these models were computed using Python. Different performance metrics were also evaluated to determine which model performed the best. Model interpretability techniques were applied to interpret the ML model.

4.2 Machine Learning Model Training and Testing Results of Loss Modulus

As mentioned in Chapter Three, 266 data were used to predict loss modulus. The data was divided into 65% for training and 35% for testing using seven inputs: binder type, temperature, frequency, shear stress, softening point, viscosity, and failure temperature to train the model. R^2, RMSE, MAE, and MAPE were determined in Table 3. to evaluate the model's predictive performance. Using scatter plots, the observed and predicted values of G" are compared by applying the three models (RF, XGBoost, and CatBoost).

Figure 3. (a) and (b) show the model performance on the training and testing set, where each model is represented using a particular marker. RF has red circles, XGBoost has blue squares and green is represented by CatBoost. For training performance, the predicted and measured have a positive linear relationship for all models. The CatBoost (green line) and XGBoost (blue line) models are closely aligned with the diagonal line indicating a strong correlation between predicted and measured G" by achieving higher accuracy with R^2 =1 than RF which deviating more from the line with the largest RMSE and MAE in term of error.

For testing, CatBoost maintains the closet's alignment with the diagonal line demonstrating a significant performance with an R^2 value of 0.9568 and a high % of MAPE from Table 3. However, RMSE and MAE were lower than the other two models. RF and XGBoost exhibit the deviation from the diagonal line with lower R^2 values of 0.882 and 0.755 respectively. In general, CatBoost demonstrated significant performance with prediction closely aligned with the diagonal line in both training and testing cases by achieving the most consistent and high performance, particularly in the training set with the highest value of R^2

and MAPE but the lowest RMSE and MAE. XGBoost comes in second position followed by RF which has less accuracy than other models.

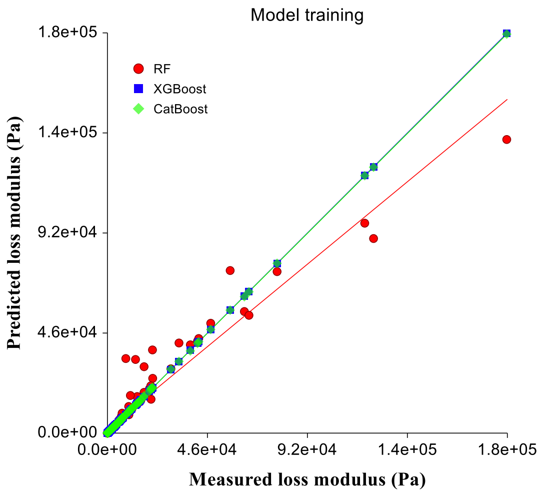
Table 3.

Fit-Accuracy Statistics of Statistical Regression Models' Prediction of Loss Modulus

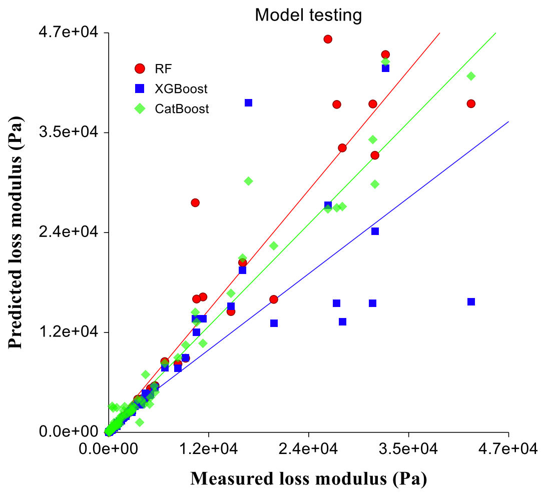
	Training			Testing		
Models	RF	XGBoost	CatBoost	RF	XGBoost	CatBoost
R^2	0.9354	1	1	0.882	0.7549	0.9568
RMSE	6554.657	1.047	163.281	5247.254	5208.924	2359.396
MAE	1899.699	0.689	123.157	1727.184	1805.779	1039.329
MAPE	10.1%	0.1%	19.5%	13.5%	14.1%	64.4%

Figure 3.

The model training and testing scatter plots between predicted and measured loss modulus for RF, XGBoost, and CatBoost models.



(a)



(b)

4.2.1 Local Effect Model Interpretation for Loss Modulus

Machine learning models are complex and challenging, often used as black boxes, while they are robust in their predictive capabilities, they provide little interpretability regarding their outputs. After modeling the two parameters (G', and G"), this research focuses on four different approaches to understanding better the models used (RF, XGBoost, and

CatBoost). These approaches include global effect (PDP) and local effect (SHAP and LIME), global importance (ICI), and local importance (PFI).

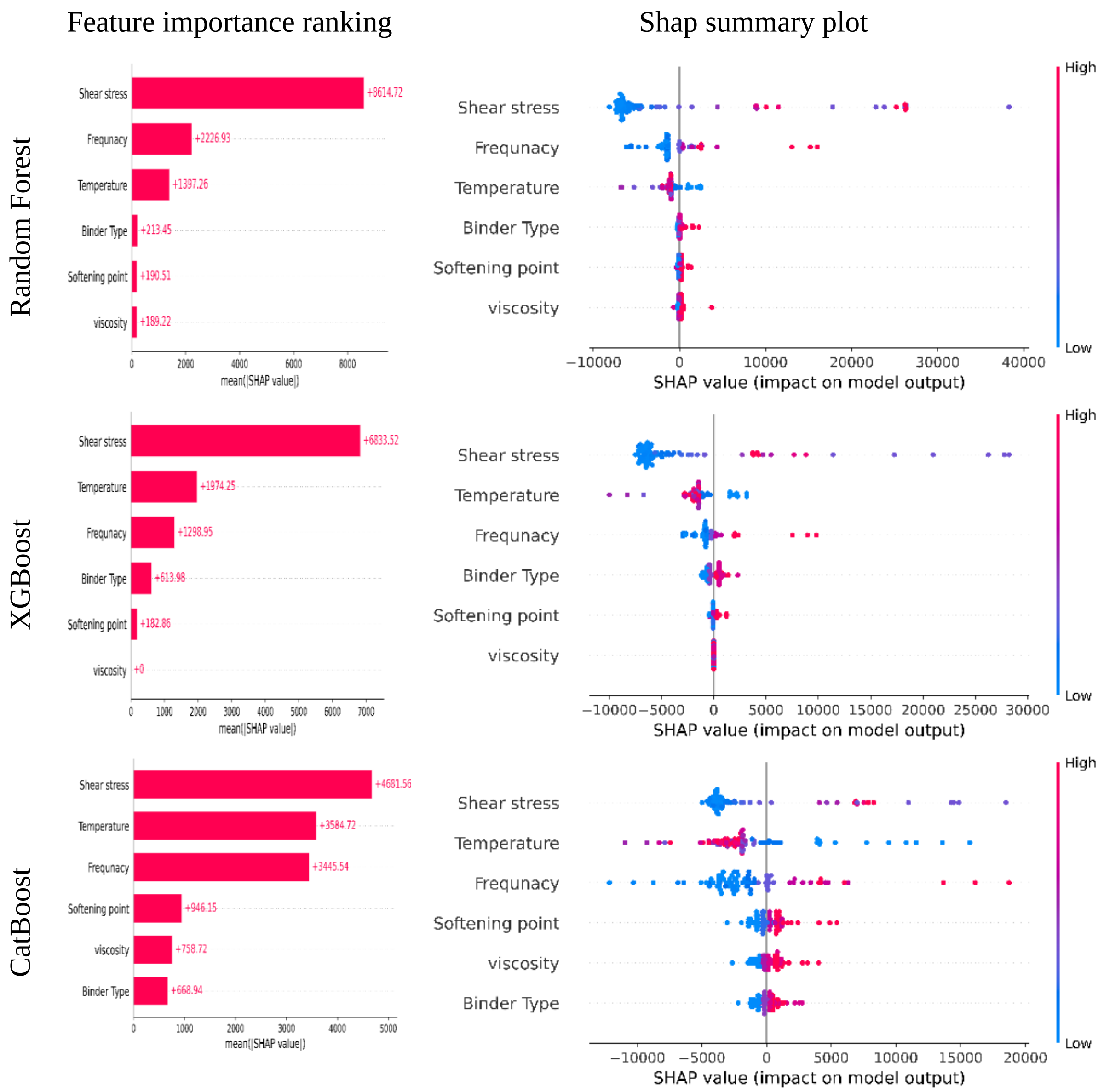
a. SHAP Value

Figure 4 illustrates feature importance ranking and SHAP summary plots for RF, XGBoost, and CatBoost using SHAP as a local effect approach to quantify the contribution of a feature for loss modulus prediction. The SHAP summary plots visualize the distribution of SHAP values for each feature by showing how the feature values affect the predictions. Six features namely shear stress, frequency, binder type, softening point, and viscosity were considered as the input variables where each dot represents a data point with its colors corresponding to the feature value: bleu represents low feature values and red suggests high feature values. The Left and right position shows whether the feature increase or decreases for the model's prediction.

On the other hand, the feature importance ranking with mean absolute SHAP values indicates the average magnitude of the impact on a feature for the model's predictions. Higher values mean the feature has a greater influence on the outputs. The result reveals that, for the Random Forest model, Shear stress has the highest mean absolute SHAP value, indicating it's the most influential feature. Frequency and Temperature also have significant impacts. The dot plot shows that higher values of Shear stress generally increase the prediction of Loss Modulus. For the XGBoost model, Similar to Random Forest, Shear stress is the most influential feature. Temperature and Frequency follow in importance. The dot plot indicates that higher Temperature values tend to decrease the prediction, while higher Frequency values increase it and for the CatBoost model, Shear stress again leads in importance. Temperature and Frequency are also significant. The dot plot for CatBoost shows a similar pattern with Shear stress and temperature impacting the prediction in opposite directions.

Figure 4.

SHAP Values of RF, XGBoost, and CatBoost for Loss Modulus

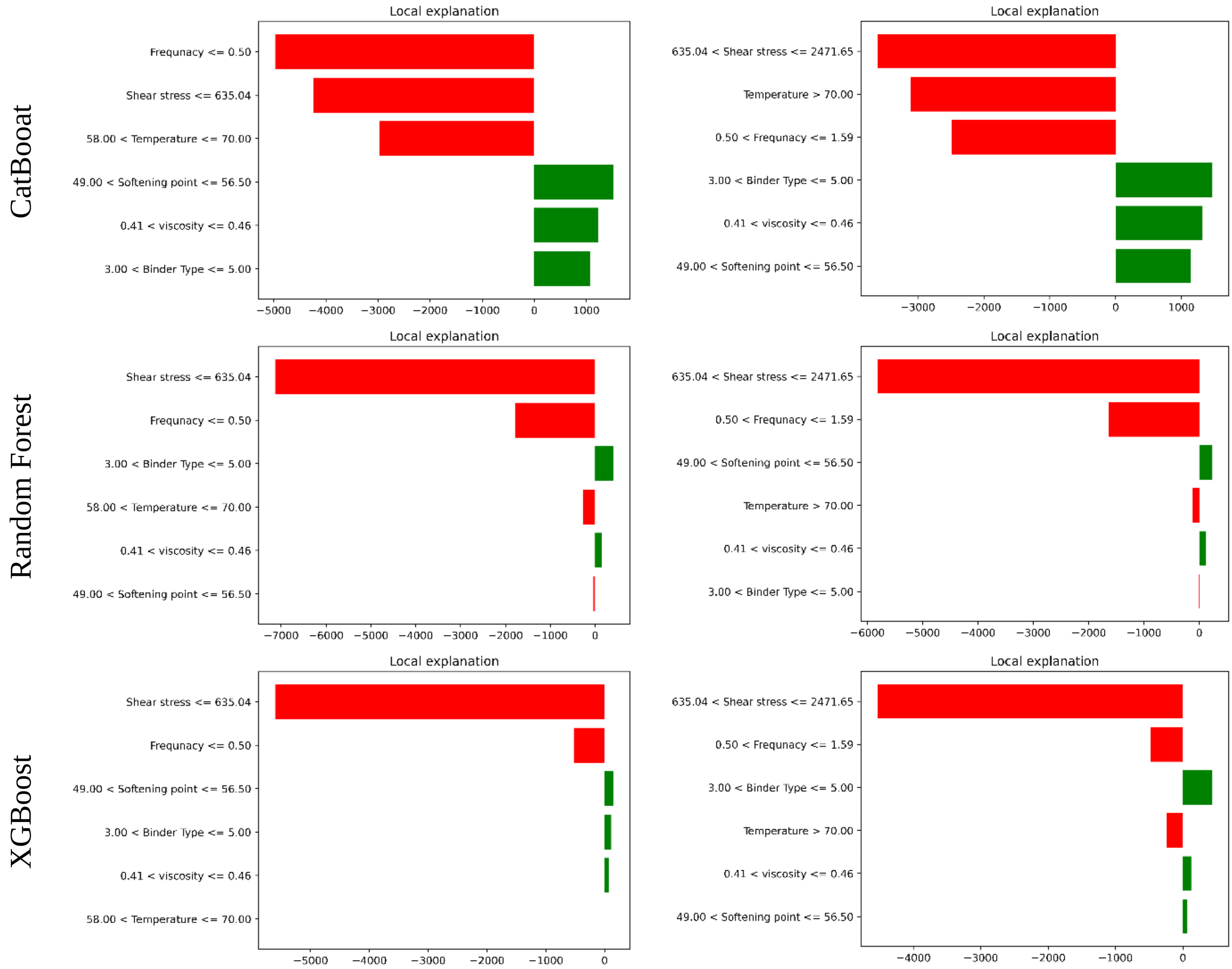


b. LIME

The Local Interpretable Model-agnostic Explanations (LIME) was used as a second approach in this research to evaluate the local effect of each feature in influence on both storage and loss modulus for 8 randomly selected instances. The figure below shows the result of LME for the three models used. For each of them, only two instances are presented in this section and six are in the appendice section. LIME values help in understanding how each feature contributes to individual predictions locally, around a specific instance. Here, the red bars represent the positive LIME values indicating features that increase the model's prediction while green bars represent the negative LIME values which indicate the features that decrease the model’s prediction. From the result, it can be observed that Shear Stress is the most influential feature across all models, with high positive LIME values indicating a significant impact on increasing the prediction of Loss Modulus followed by frequency which has also a notable impact, with positive LIME values in most models, suggesting it generally increases the prediction. Temperature varies in impact but often has a significant positive effect, though in some models, it might have a lesser impact compared to other features in addition, the softening point generally has a smaller but still notable impact, with positive LIME values. Finally, viscosity: Often has the least impact on the prediction of Loss Modulus, indicated by lower LIME values, and, binder type varies in impact, with some models showing it as more influential than others.

Figure 5.

LIME Values of RF, XGBoost, and CatBoost for Loss Modulus



For Random Forest, shear stress is the dominant feature, followed by Frequency and Temperature. The impact of Binder Type and Softening Point is less pronounced but still present. In the XGBoost model again, Shear stress leads in importance. Frequency and Temperature follow, with Temperature having a mixed impact. The softening point and viscosity have lesser impacts, with viscosity being the least influential. For CatBoost, similar pattern with Shear stress being the most influential. Frequency and Temperature are also significant but show varied impacts. Softening Point and Viscosity have smaller impacts, with viscosity being the least influential

4.2.2 Local importance model interpretation for loss modulus

The local importance analysis was evaluated using the Individual Conditional Importance (ICI) approach for different features with average ICI for the Top 100% of Instances (All Test Set) (left plots) and ICI for Selected Instances (right plots) of three models when predicting the loss modulus. The ICI plots illustrated in Figure 6 are used to interpret the performance of the machine learning model.

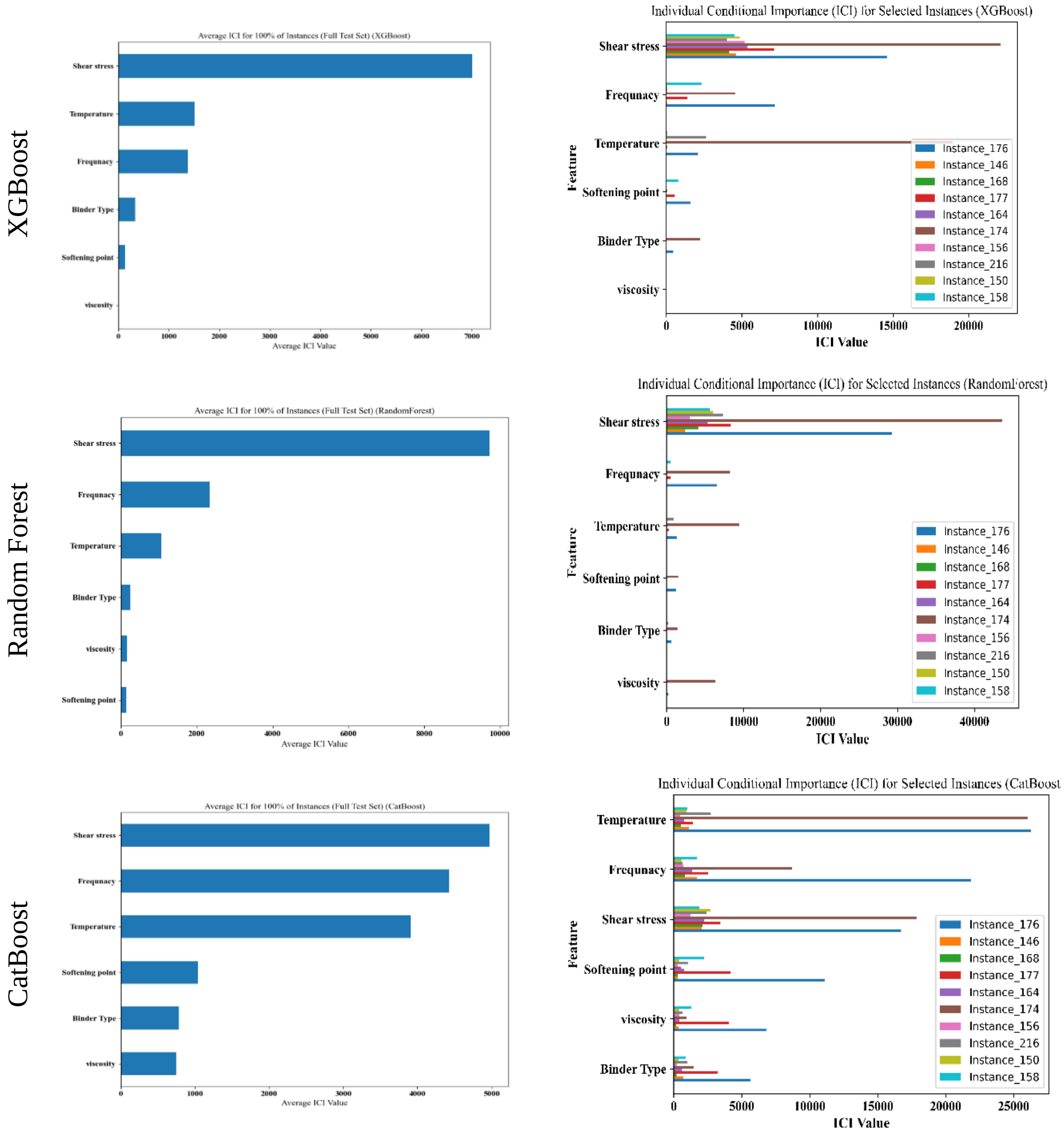
For XGBoost, shear stress is the most important feature with high values of ICI across all instances, indicating that it is a crucial feature when predicting loss modulus, followed by temperature but this shows variability across instances. Frequency is also a third important feature but less than the first two top ones. Its importance varies, meaning it interacts with other features. Softening point, binder type, and viscosity have lower values of ICI this means that they are less critical features with lower importance but they still contribute to the model.

For the Random Forest model, shear stress again is the most important feature, indicating its critical role in predictions. The consistency across instances confirms its significance. Temperature is important but not as much as Shear Stress. The variability in its importance across instances suggests it might not always be a decisive factor. Frequency shows some importance but less than temperature, indicating it might be less universally applicable or its effect might be weak in certain conditions. In contrast to XGBoost, the softening point, binder type, and viscosity characteristics seem to be even less significant in this model. This suggests that because Random Forest incorporates several decision trees, these qualities may not be as important in Random Forest or their influence may be depicted differently.

As demonstrated by its consistent importance across models, shear stress is still the most important parameter in the CatBoost model for forecasting Loss Modulus. In other situations, temperature is found to be highly significant, indicating that its effects may be more situation-specific. In comparison to other models, frequency is also very important, which may suggest a more important or subtle role for CatBoost. The importance of viscosity, binder type, and softening point vary; in certain cases, these characteristics are more important than others. This fluctuation may suggest that, depending on their interactions with other variables or the particular context of the prediction, certain features may occasionally be crucial inside the CatBoost framework.

Figure 6.

ICI Values of RF, XGBoost, and CatBoost for Loss Modulus



4.2.3 Global Effect Model Interpretation for Loss Modulus

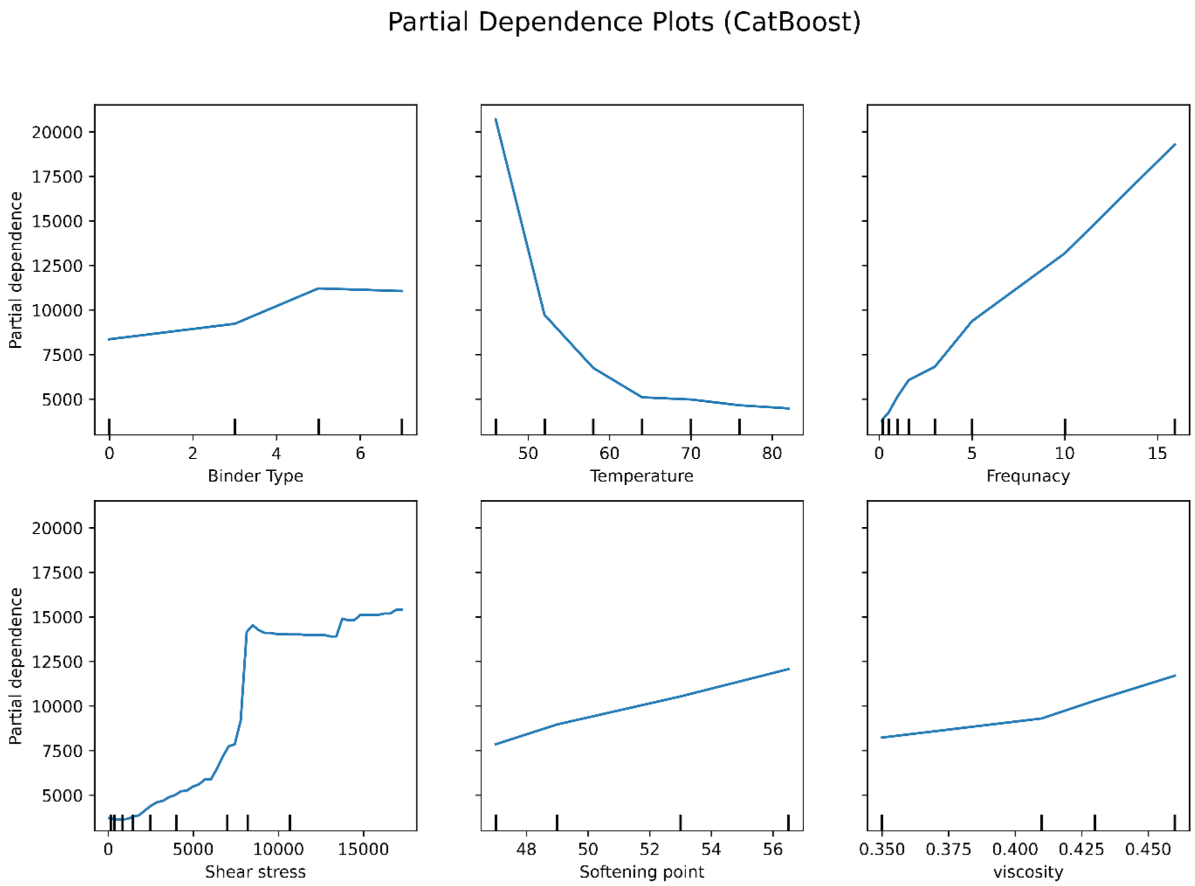
The three models were interpreted using a global effect method called the Partial Dependency Plot (PDP). By averaging the effects of all features, PDP enables us to comprehend the relationship between each feature and the anticipated loss or storage modulus. It can examine how modifications to a single feature may impact the model's prediction.

The x-axis represents the range for feature value, while the y-axis indicates the effect of the feature on the prediction. The curves on PDP illustrated how predictions change in the model’s prediction as the feature value changes. If the curve rises as you move along the x-axis, it means that increasing the feature's value results in higher predictions from the model, If the curve falls or downward slope, it indicates that increasing the feature's value leads to lower predictions. A horizontal or flat PDP curve suggests that changes in the feature's value do not significantly affect the model's predictions.

For the CatBoost model, the plot in Figure 7. shows a gradual increase in the partial dependence as the Binder Type value increases. This indicates that higher binder-type values tend to increase the predicted Loss Modulus. However, there is a noticeable decrease in the partial dependence as the temperature increases from around 50 to 70. This suggests that the Loss Modulus prediction decreases with increasing temperature up to a certain point, after which it stabilizes. The partial dependence increases linearly with frequency and sharply with the shear stress up to around 5000, followed by a rise curve. This implies that higher frequencies and shear stress values significantly increase the predicted Loss Modulus, but the effect diminishes after a certain point for shear stress. Furthermore, there is a little upward trend as viscosity and softening point rise, suggesting that greater values of these two characteristics result in somewhat larger Loss Modulus estimates.

Figure 7.

PDP Values of CatBoost for Loss Modulus



The PDP results for the Random Forest (RF) and XGBoost models are presented in Figures 8 and 9. The results indicate that for the RF model, the loss modulus increases slightly with rising binder types. Conversely, the plot demonstrates a downward trend concerning temperature, showing that the loss modulus decreases as temperature increases. There is also a modest upward trend in loss modulus with increasing frequency, indicating that higher frequency leads to an increase in the loss modulus. Additionally, there is a sharp increase in G" as the shear stress approaches 10000, after which it stabilizes. The softening point and viscosity have little to no significant effect on the loss modulus.

For XGBoost, loss modulus behaves a little differently as shown in Figure 9, where it remains relatively constant for lower binder types but increases slightly with higher binder types, indicating a minor positive effect. G" decreased as the temperature rises beyond 60 C, showing a strong negative impact of higher temperatures on predictions. Similar to storage modulus, G" increases with frequency in a linear pattern. There is a sharp and consistent increase in G" with increasing shear stress, particularly at lower levels. G" decreases slightly with increasing softening points, showing a weak negative impact. There is no influence in viscosity because G" remains unaffected by changes.

Figure 8.

PDP Values of Random Forest for Loss Modulus

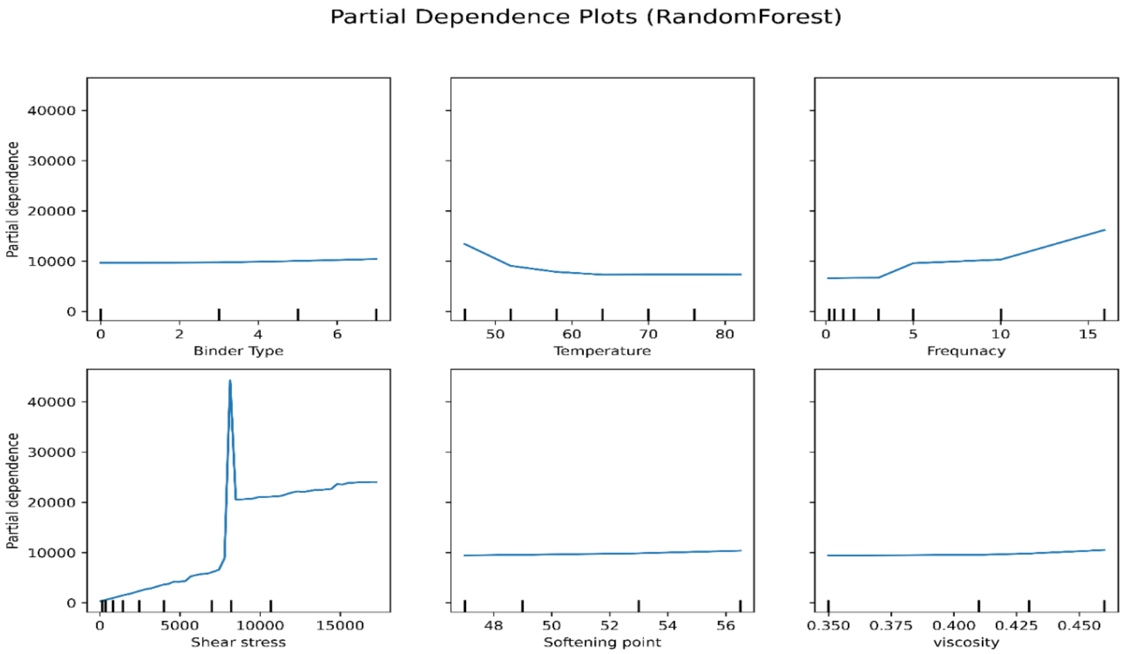
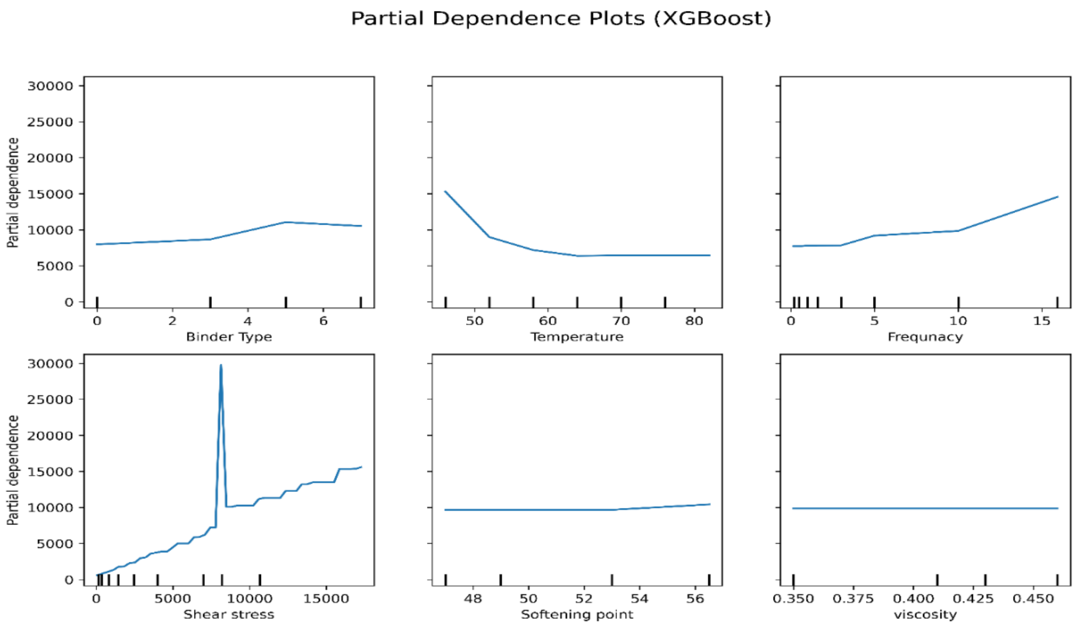


Figure 9.

PDP Values of XGBoost for Loss Modulus



4.2.4 Global Importance Model Interpretation for Loss Modulus

Permutation Feature Importance (PFI) analysis was used in this research to identify the most significant features of each model for the prediction of both loss and storage modulus. Here are the results of the three models for loss modulus illustrated in subplots a,b, and c expressed as the mean decrease in accuracy:

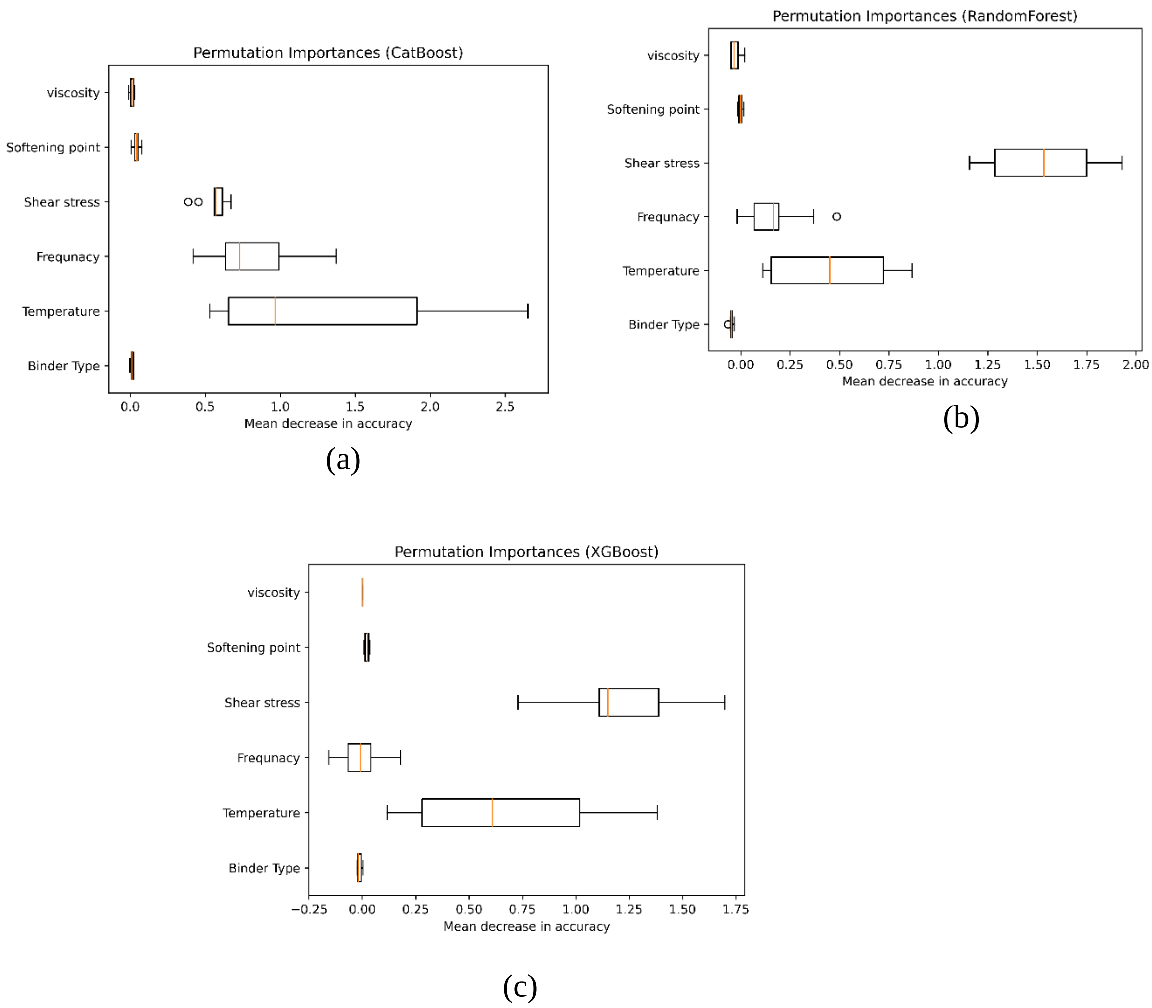
In Figure (a), for CatBoost permutation importance, temperature is the most important feature, with the highest mean decrease in accuracy when permuted, followed by frequency and shear stress with less impact than temperature. Softening point and viscosity have very small mean decreases, meaning that they have a minimal contribution to the model's accuracy. The binder type is the smallest important feature, showing negligible impact.

In Figure (b), Random Forest model, shear stress is the most important feature, followed by temperature, but its impact is lower compared to the shear stress, and frequency ranked third. Softening point and viscosity both have minimal influence, similar to CatBoost and binder type again is the last with no impact. In Figure (c), for XGBoost, temperature dominates as the most important feature, similar to CatBoost, followed by shear stress and frequency. Softening point and viscosity have less impact, comparable to the other models, and binder type is still negligible.

It can be observed that temperature and shear stress were the most important features and varied between models, with XGBoost and CatBoost ranking temperature, while RF was shearing stress, and across all the models, frequency ranks third influential feature. The softening point, viscosity, and binder type have less contribution.

Figure 10.

Permutation Feature Importance (PFI) analysis of (a) CatBoost, (b) Random Forest, and (c) XGBoost for loss modulus prediction



4.3 Machine Learning Model Training and Testing Results of Storage Modulus

266 data were used again for the prediction of storage modulus G' and divided into 65% for training and 35% for testing. However, seven inputs were used to train the model which were the six previous plus the failure temperature. The same metrics are also used in Table 4. to evaluate the model's predictive performance. Using scatter plots, the observed and predicted values of G' are compared by applying the same models (RF, XGBoost, and CatBoost).

In training, all models show a strong positive correlation between predicted and actual values, with data points closely aligned along the diagonal, indicating good model fit. XGBoost and CatBoost achieved a perfect score with an R^2 value of 1 than RF which was slightly lower but still very high as shown in Figure 11. XGBoost had the lowest RMSE, MAE, and MAPE values of 0.298, 0.209, and 1.6% respectively.

The model testing shows more variation, especially for the RF and XGBoost model, which shows a deviation from the diagonal line. This indicated that while the models work well overall, they are not as precise as they were during training. In contrast, CatBoost predictions are closer to the diagonal line than the others, indicating it has better accuracy with an R^2 value of 0.9062 and the lowest error metrics with values of 542.064 and 198.703 for RMSE and MAE respectively.

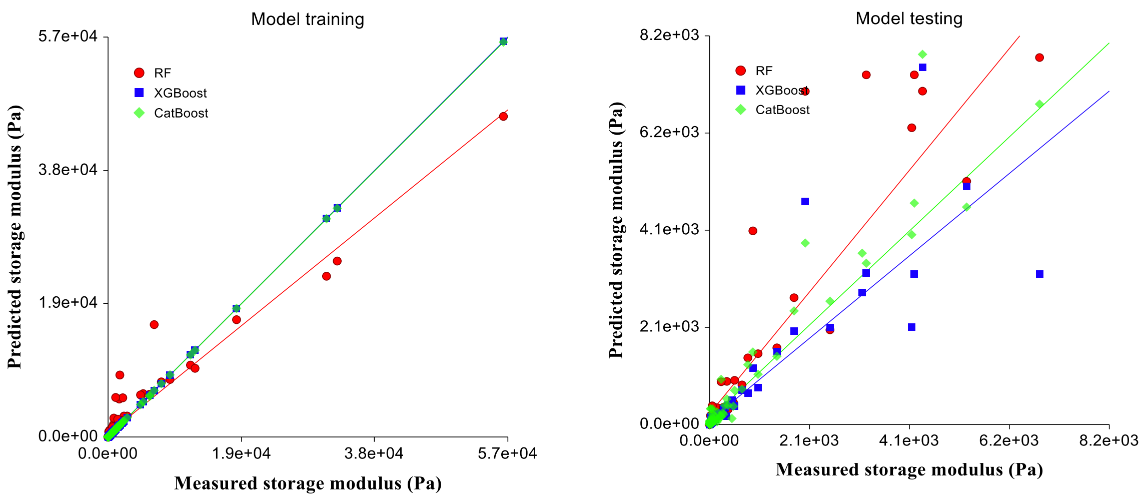
Table 4.

Fit-Accuracy of Statistical Regression Models' Prediction of Storage Modulus

	Training			Testing		
Models	RF	XGBoost	CatBoost	RF	XGBoost	CatBoost
R^2	0.9392	1	1	0.7526	0.8332	0.9062
RMSE	1761.531	0.298	37.285	1362.277	697.476	542.064
MAE	535.01	0.209	25.969	462.643	220.748	198.703
MAPE	38.4%	1.6%	169.9%	69.4%	38.8%	498.6%

Figure 11.

The model training and testing scatter plots between predicted and measured storage modulus for RF, XGBoost, and CatBoost models



4.3.1 Local Effect Model Interpretation for Storage Modulus

a. SHAP values

In the predicting storage modulus, the result of each model demonstrated that, for Random Forest, Similarly, to loss modulus, shear stress remains the most important feature with the largest mean SHAP value. Temperature and frequency are next followed by softening point, binder type, and viscosity with smaller contributions for G'. On the other hand, SHAP summary plots demonstrated that shear stress has a significant positive influence on the model FR model, although G's prediction, has some negative consequences that tend to decrease the prediction. Temperature and frequency affect positively predictions, but their impact is less than that of shear stress. The softening point, binder type, and viscosity have a smaller but still noticeable effect, with high values contributing positively in most cases.

For XGBoost, the feature importance is ranked and we can see that shear stress has the largest mean SHAP value making it the most important feature, followed by temperature and frequency. Binder type and softening point contribute minimally, consistent with the results from the Random Forest (RF) model. Interestingly, viscosity shows no impact on the XGBoost predictions, which contrasts with the other two models, where it had a small positive contribution. While the summary plot illustrated that shear stress consistently increases the predictions of G'. High temperatures still decrease the predicted storage modulus while high-frequency values increase the storage modulus. Although binder type and softening point show higher values, indicating they also contribute positively, their influence is less than that of the top three features. The lack of viscosity influence in XGBoost suggests it may not capture minor dependencies as effectively as RF.

For the CatBoost model, temperature is the top feature with the higher mean SHAP value, indicating a strong influence on the model’s prediction, with high temperature reducing the storage modulus, followed by shear stress and frequency. Softening point, viscosity, and binder type have lower SHAP values with a small impact compared to other features.

Figure 12.

SHAP Values of RF, XGBoost, and CatBoost for Storage Modulus

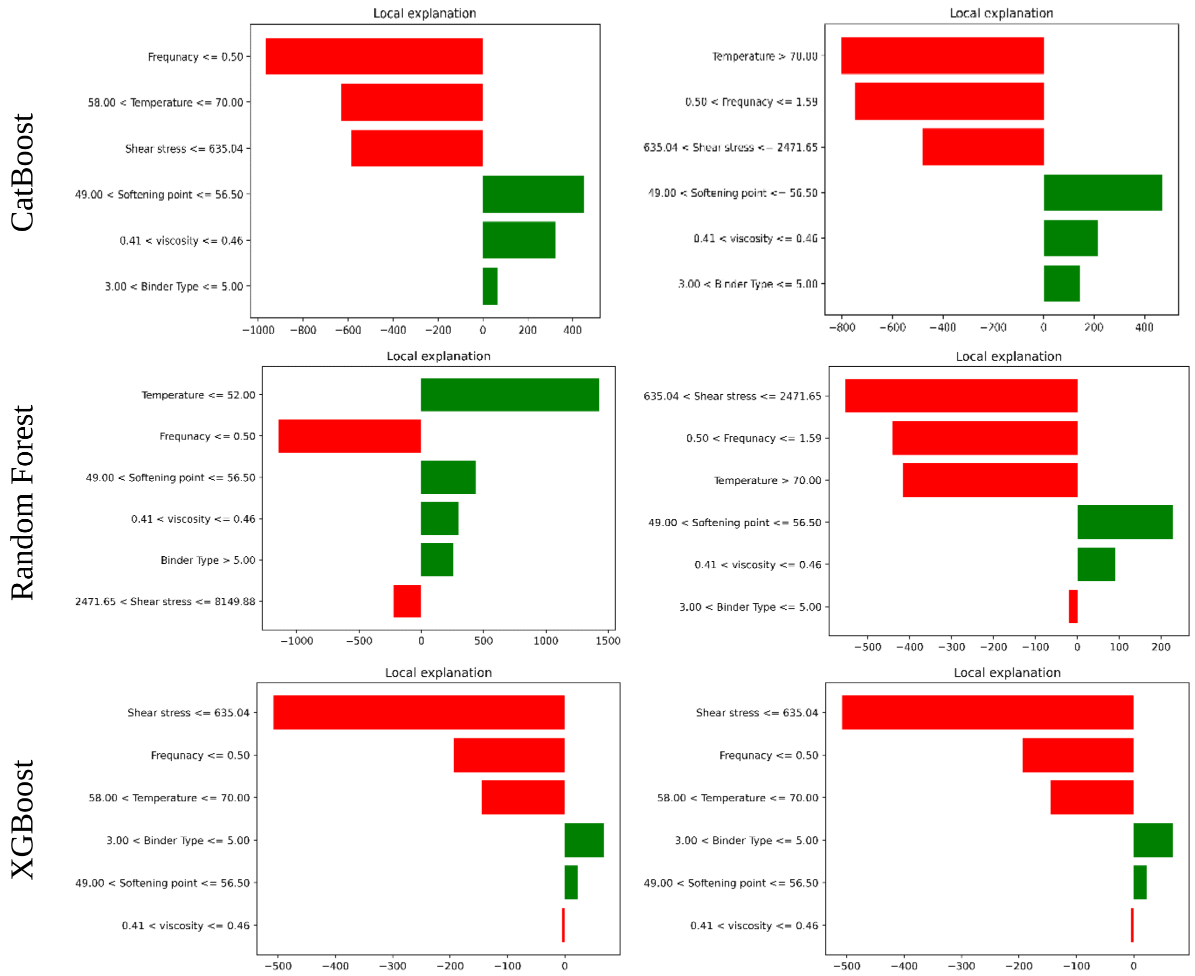
b. Local Interpretable Model-agnostic Explanations (LIME)

CatBoost seems to place high importance on temperature and shear stress for predicting storage modulus, with Temperature's effect being more pronounced in the left plot instance and Shear Stress in the right plot instance. Frequency has a consistently negative but small effect while the Softening point shows a positive impact in both plots. However, viscosity and binder type have a minor negative impact on the model’s prediction.

Random Forest relies heavily on Shear Stress for both instances, indicating it's a dominant feature. Temperature has a significant but variable impact, being negative in both instances but more so in the right plot. Frequency shows a slight shift from negative to positive impact, suggesting variability in its influence. XGBoost consistently highlights Shear Stress and Temperature as key positive contributors to the storage modulus prediction. Frequency consistently has a minor negative impact across both instances, indicating a stable influence pattern.

Figure 13.

LIME Values of RF, XGBoost, and CatBoost for Storage Modulus



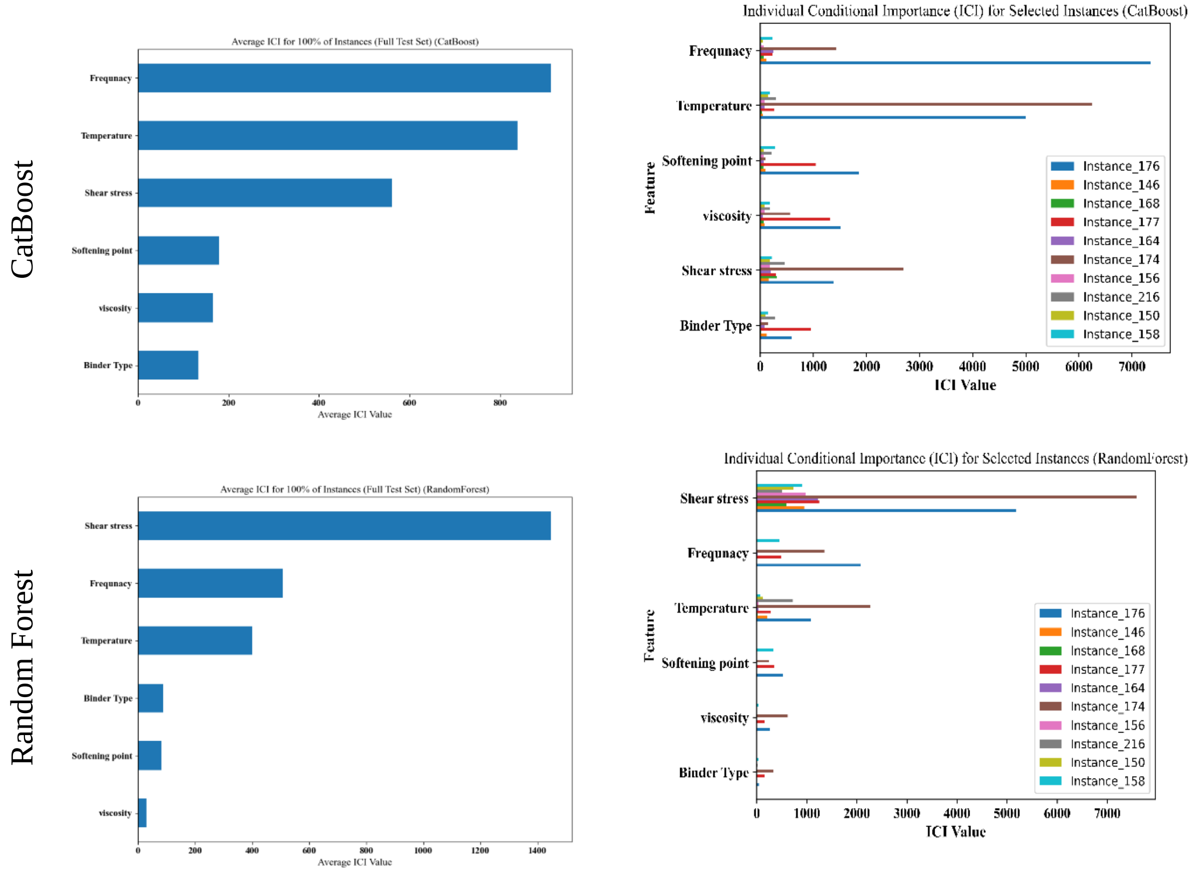
4.3.2 Local importance model interpretation for storage modulus

In the prediction of storage modulus, the result demonstrated that for the XGBoost model, shear stress, temperature, and frequency are the most important features, indicating a strong influence on the storage modulus. Softening point and binder type have lower importance but they still have a considerable role in the model's prediction. Viscosity has no ICI value, meaning that it is not an important feature and does not contribute to the model's prediction. In terms of selected instances, the variation in ICI values across instances for each feature, particularly for shear stress, temperature, and frequency, indicates that while these features are generally important, their impact can vary significantly depending on the specific context of each instance. This suggests potential interactions or dependencies among features.

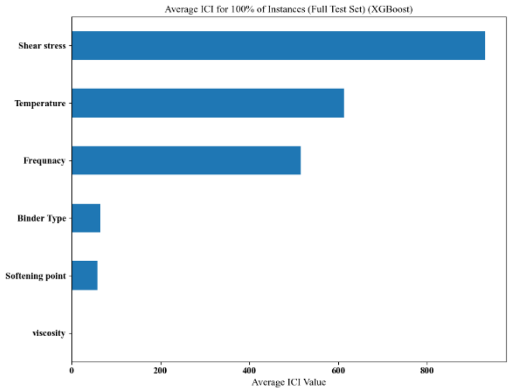
For Random Forest, shear stress, frequency, and temperature are the major predictor features while, softening point, binder type, and viscosity still have lower importance with a contribution to the model. The lines illustrated in the right plot show variability in importance across instances, particularly for Shear Stress and Frequency. This could imply that the model's predictions are sensitive to the specific combinations of these features in different instances, highlighting potential feature interactions or instance-specific effects.

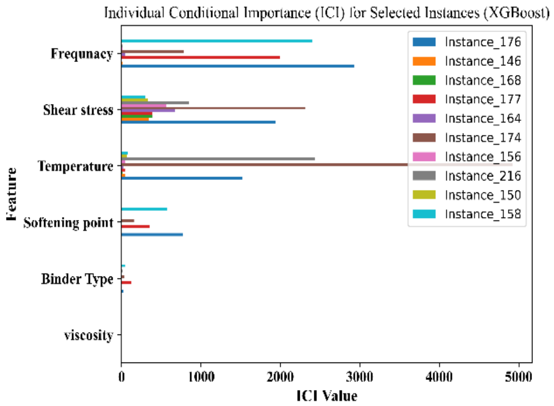
Figure 14.

Values of RF, XGBoost, and CatBoost for Storage Modulus



XGBoost





In CatBoost, features behave a little differently, where frequency is the most important, followed by temperature and shear stress which are less important than in the other models. This might reflect how the CatBoost model processes and weights features. The three last features remain the same with lower importance but still contribute. The individual lines for different instances show that frequency consistently has high importance across all instances, with temperature and shear stress showing variability.

4.3.3 Global Effect Model Interpretation for Storage Modulus

Figure 15. Shows the result of PDP of XGBoost for storage modulus prediction and the result reveals that, G' increases with the binder type, showing that changes in binder type have a small effect on predictions. At lower temperatures, G' remains stable. However, when the temperature goes above 60°C, G' begins to decrease rapidly, indicating a strong negative impact at high temperatures. G' also increases linearly with frequency, meaning higher frequencies improve predictions. There is a steep rise in G' with increased shear stress, especially at lower levels, which indicates a strong positive relationship. G' increases slightly with the softening point, indicating a weak positive correlation, while viscosity has little effect, as G' stays nearly constant regardless of changes in viscosity.

For Random Forest, the storage modulus slightly increases as the binder type rises, but the effect is minor and less pronounced as shown in Figure 16. It significantly decreases with the temperature but has a positive effect frequency because it steadily increases. Shear stress is a dominant factor in predictions, this is because G' increases sharply as shear stress rises, especially in the lower range. G' slightly increases with the softening point and viscosity but the effect is little.

For the CatBoost model, figure 17. illustrated that the storage modulus shows a slight upward trend as the binder type increases, indicating a minor positive effect. There is a significant decline in G' with increasing temperature, but a strong positive relationship is observed between frequency and storage modulus, with higher frequencies leading to higher G' values. G' increases steadily as shear stress rises, with a sharper increase in the lower range, making shear stress one of the dominant factors. It shows a slight increase with the softening point. There is a slight upward trend in storage modulus as viscosity increases, suggesting a minor positive effect.

Figure 15.

PDP Values of XGBoost for Storage Modulus

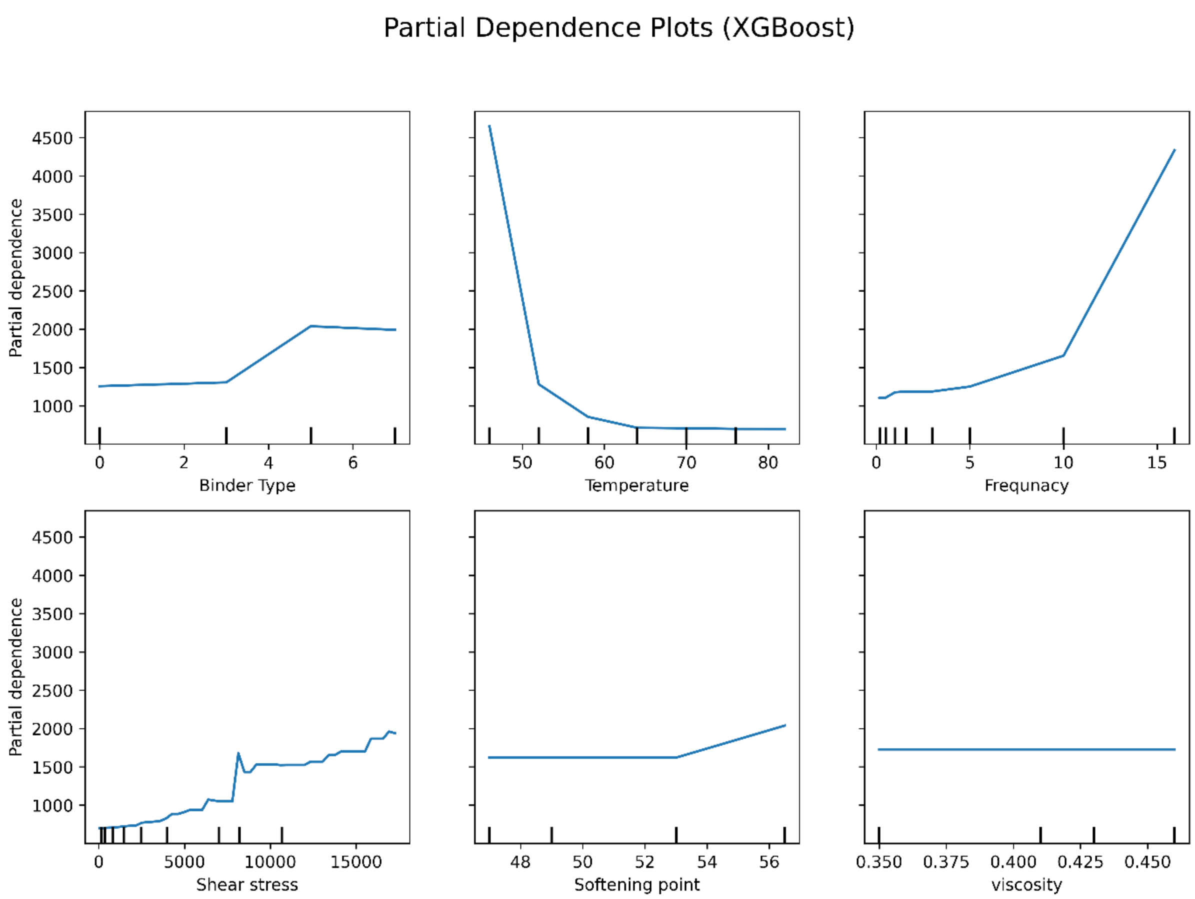


Figure 16.

PDP Values of Random Forest for Storage Modulus

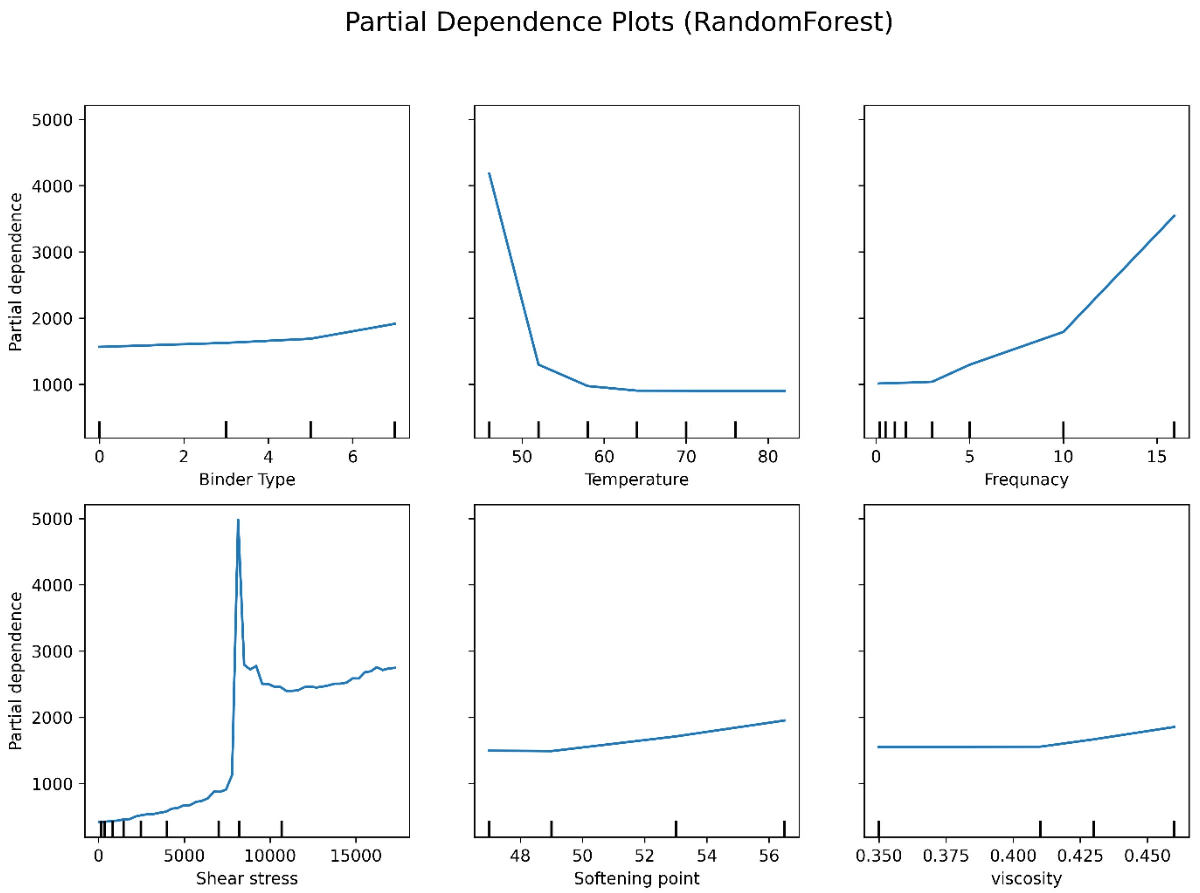
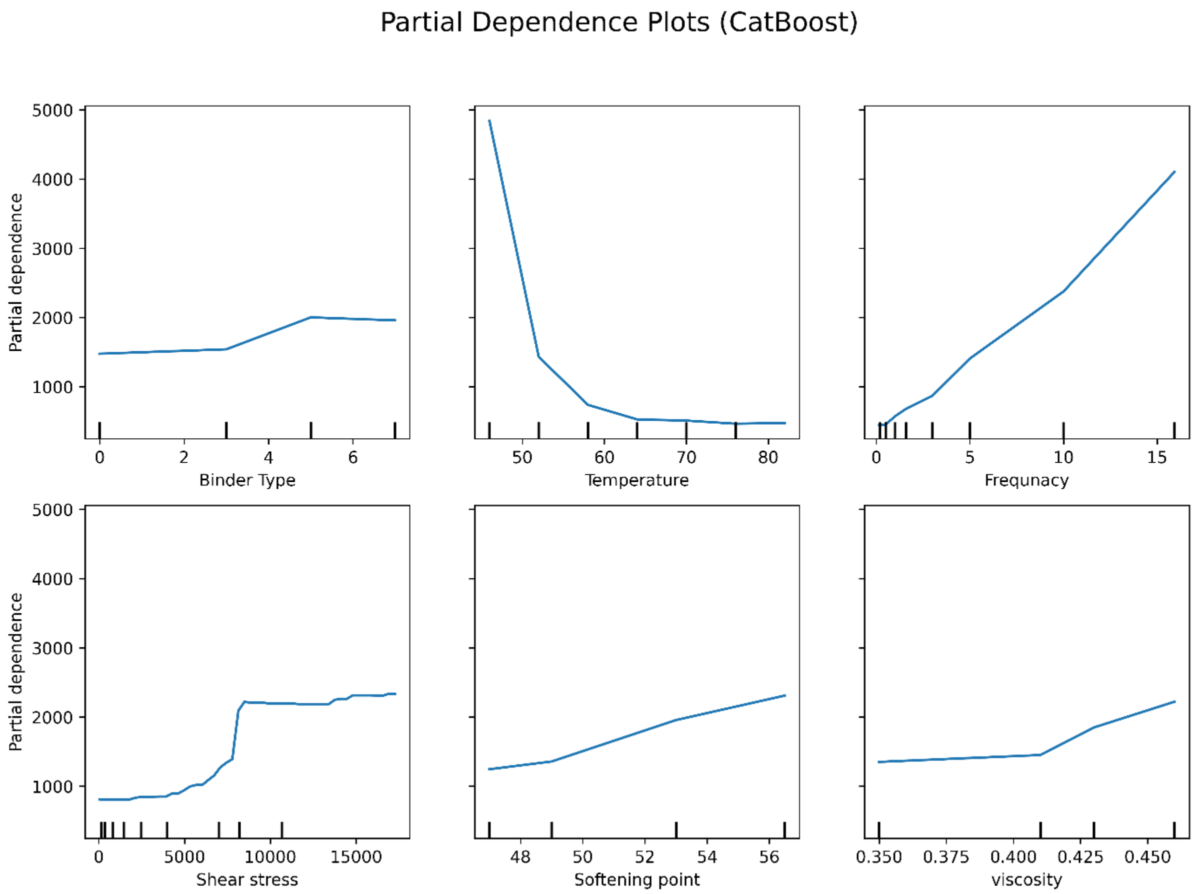


Figure 17.

PDP Values of CatBoost for Storage Modulus



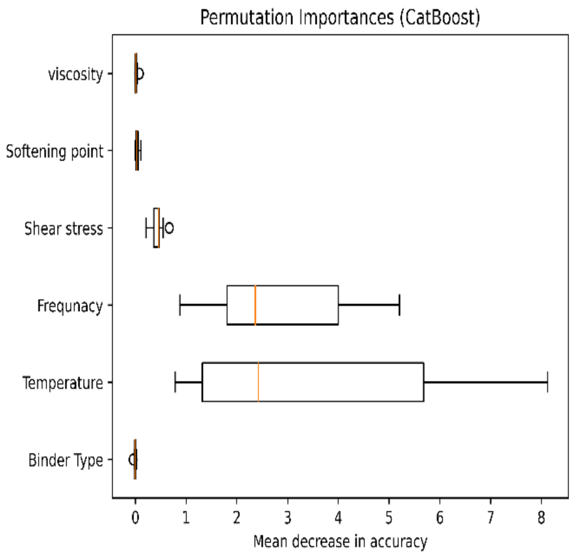
4.3.4 Global Importance Model Interpretation For Storage Modulus

Permutation Importance plots are represented in Figure 18 (a-c) for different machine learning models in predicting storage modulus. Here are the results of each model:
For CatBoost, as shown in Figure (a), temperature is the most important feature, with a strong significant mean decrease in accuracy when permuted, followed by frequency, with moderate importance. Shear stress ranked third with a smaller mean decrease accuracy but a notable impact. Softening point and viscosity have minimal contribution to the model's accuracy and binder type is the last important feature, with almost no influence on the prediction.

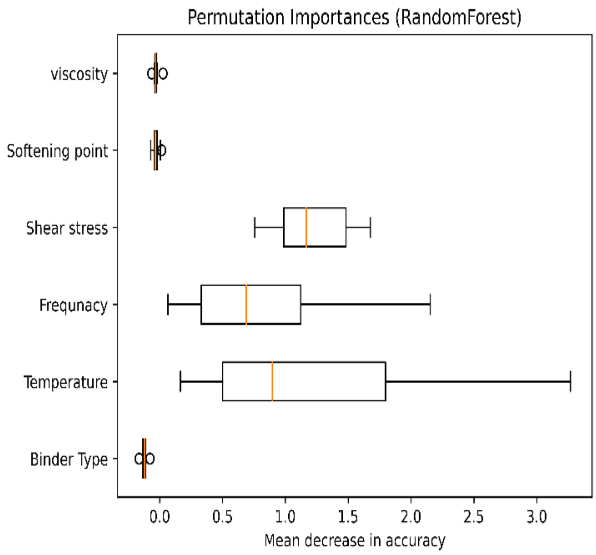
In Figure (b), for the Random Forest model, temperature is the most important variable and consistently crucial across the RF model followed by frequency. Shear stress has a moderate influence similar to frequency but slightly lower. Softening point, viscosity, and binder type were similar to Loss Modulus showing negligible influence. For XGBoost permutation importance, in Figure (c), temperature, frequency, and shear stress ranked as the most influential features. Softening point and viscosity have little contribution, with very low mean decreases in accuracy and binder type has negligible importance. For storage modulus prediction, temperature shows the highest impact on predictions in all three models and is the most important feature across all models. Followed by frequency and shear stress mean that they are second feature contributors. The softening point, viscosity, and binder type have little impact in all models, suggesting they are not crucial for predicting storage modulus in this dataset.

Figure 18.

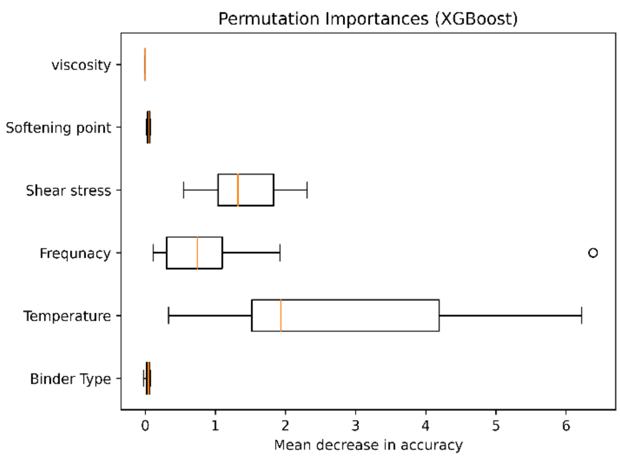
Permutation Feature Importance (PFI) analysis of (a) CatBoost, (b) Random Forest, and (c) XGBoost for Storage Modulus prediction



(a)



(b)



(c)

Chapter V

Conclusion and Recommendations

5.1 Conclusion

This research focused on the prediction of storage modulus and loss modulus of modified asphalt binders. For this purpose, three different machine learning techniques namely Random Forest, XGBoost, and CatBoost were developed using the Python tool. Due to a lack of insufficient model interpretation, the research utilized the model interpretability approach to interpret the predictions of the used machine learning models by providing insights into the feature's contributions and their impact on the model's prediction at local and global levels.
The computational models were evaluated using four different performance criteria: R^2 (coefficient of determination), RMSE (Root Mean Square Error), MAE (Mean Absolute Error), and MAPE (Mean Absolute Percentage Error), after modelling, CatBoost outperformed other models (RF and XGBoost) in predicting the loss modulus (G") and storage modulus (G') for both training and testing datasets. It achieved the highest R^2 and MAPE values, with the lowest RMSE and MAE, indicating its superior accuracy and prediction consistency.

LIME (Local Interpretable Model-agnostic Explanations), SHAP (Shapley Additive explanations), ICI (Interaction-based Contribution Index), PDP (Partial Dependence Plots), and PFI (Permutation Feature Importance were analyzed to identify the effect and importance of features that contribute significantly to the model's predictions. The result indicated that shear stress and temperature emerged as the most influential and significant features across all models, since they positively impact the predictions of both storage and loss modulus, followed by frequency which contributes less than the other two features. The softening point, binder type, and viscosity were found to have negligible contributions to the model's prediction, but they had a positive impact.

It was also noticed that the temperature played a crucial role in predicting storage and loss modulus across all model, whereas temperature increases, both G', and G" decrease, emphasizing the importance of temperature control in applications involving geopolymer-modified asphalt binders. Similarly, viscosity shows no influence in the XGBoost model.

5.2 Recommendation

For the performance of high temperature in predicting Storage and Loss modulus, the CatBoost model should be prioritized since it demonstrated the best performance. Based on the result, future research should focus on the most influential features identified across the model including shear stress, temperature, and frequency to enhance prediction accuracy. It is crucial to control temperature during experiments since it impacts the model's prediction.

References

Ali, S. I. A., Yahia, H. A. M., Ibrahim, A. N. H., & Al Mansob, R. A. (2017). High temperatures performance investigation of geopolymer modified bitumen binders. *Bearing Capacity of Roads, Railways and Airfields - Proceedings of the 10th International Conference on the Bearing Capacity of Roads, Railways and Airfields, BCRRA 2017, June*, 417–422. https://doi.org/10.1201/9781315100333-60

Arfat, M., Yaacob, H., Hassan, N. A., Warid, M. N. M., Idham, M. K., Ismail, C. R., Nor, H. M., Hainin, M. R., Mohamed, A., Mashros, N., Yunus, N. Z. M., Hassan, S. A., Jaya, R. P., & Ayob, M. F. (2019). Reversible moisture damage in asphalt mixture. *IOP Conference Series: Materials Science and Engineering*, *527*(1). https://doi.org/10.1088/1757-899X/527/1/012057

Ayazi, M. F., Singh, M., & Kumar, R. (2024). Prediction and modelling marshall stability of modified reclaimed asphalt pavement with rejuvenators using latest machine learning techniques. *Engineering Research Express*, *6*(3). https://doi.org/10.1088/2631-8695/ad65b7

Bennert, T., Garg, N., Ericson, C., & Cytowicz, N. (2023). Evaluation of Test Methods to Identify Asphalt Binders Prone to Surface-initiated Cracking. *Transportation Research Record*, 897–910. https://doi.org/10.1177/03611981221119191

Bi, Y., Xiang, D., Ge, Z., Li, F., Jia, C., & Song, J. (2020). An Interpretable Prediction Model for Identifying N7-Methylguanosine Sites Based on XGBoost and SHAP. *Molecular Therapy Nucleic Acids*, *22*(December), 362–372. https://doi.org/10.1016/j.omtn.2020.08.022

Botella, R., Lo Presti, D., Vasconcelos, K., Bernatowicz, K., Martínez, A. H., Miró, R., Specht, L., Mercado, E. A., Pires, G. M., Pasquini, E., Ogbo, C., Preti, F., Pasetto, M., del Barco Carrión, A. J., Roberto, A., Orešković, M., Kuna, K. K., Guduru, G., Martin, A. E., … Tebaldi, G. (2022). Machine learning techniques to estimate the degree of binder activity of reclaimed asphalt pavement. *Materials and Structures/Materiaux et Constructions*, *55*(4). https://doi.org/10.1617/s11527-022-01933-9

BREIMAN, L. (2001). *Random Forests*.

Brenning, A. (2023). Interpreting machine-learning models in transformed feature space with an application to remote-sensing classification. *Machine Learning*, *112*(9), 3455–3471. https://doi.org/10.1007/s10994-023-06327-8

Bujang, H., Aman, M. Y., Arumugam, T. N., & Taher, M. N. M. (2023). Physical Characterization of Modified Asphalt Binder with Differing Fly Ash Geopolymer Contents. *International Journal of Integrated Engineering*, *15*(1), 331–338. https://doi.org/10.30880/ijie.2023.15.01.030

Bujang, H., Aman, M. Y., & Taher, M. N. M. (2022). Volumetric Properties of Asphalt Mixture Containing Fly Ash Geopolymer. *IOP Conference Series: Earth and Environmental Science*, *1022*(1). https://doi.org/10.1088/1755-1315/1022/1/012034

Bujang, H., Aman, M. Y., Taher, M. N. M., & Suradi, S. S. (2023). Effects of Fly Ash

Geopolymer Hot Mix Asphalt Additive on the Rheological Properties of Unaged and Short-Term Aged Asphalt Binder. *Journal of Advanced Research in Applied Mechanics, 109*(1), 44–52. https://doi.org/10.37934/aram.109.1.4452

Casalicchio, G., Molnar, C., & Bischl, B. (2019). Visualizing the feature importance for black box models. *Lecture Notes in Computer Science (Including Subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics), 11051 LNAI*, 655–670. https://doi.org/10.1007/978-3-030-10925-7_40

Chen, T., & Guestrin, C. (2016). XGBoost: A scalable tree boosting system. *Proceedings of the ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, 13-17-Augu*, 785–794. https://doi.org/10.1145/2939672.2939785

Cheng, X., Liu, Y., Ren, W., & Huang, K. (2019). Performance evaluation of asphalt rubber mixture with additives. *Materials*, *12*(8). https://doi.org/10.3390/ma12081200

Cheng, Y., Li, L., Zhou, P., Zhang, Y., & Liu, H. (2019). Multi-objective optimization design and test of compound diatomite and basalt fiber asphalt mixture. *Materials, 12*(9). https://doi.org/10.3390/ma12091461

Dalwinder Singh and Birmohan Singh. (2020). Investigating the impact of data normalization on classification performance. *Applied Soft Computing Journal*.

Diab, A., Enieb, M., & Singh, D. (2019). Influence of aging on properties of polymer-modified asphalt. *Construction and Building Materials*, *196*, 54–65. https://doi.org/10.1016/j.conbuildmat.2018.11.105

Dindorf, C., Teufl, W., Taetz, B., Bleser, G., & Fröhlich, M. (2020). Interpretability of input representations for gait classification in patients after total hip arthroplasty. *Sensors (Switzerland)*, *20*(16), 1–14. https://doi.org/10.3390/s20164385

Dong, W., Ma, F., Li, C., Fu, Z., Huang, Y., & Liu, J. (2020). Evaluation of anti-aging performance of biochar modified asphalt binder. *Coatings*, *10*(11), 1–19. https://doi.org/10.3390/coatings10111037

Dorogush, A. V., Ershov, V., & Gulin, A. (2018). *CatBoost: gradient boosting with categorical features support*. 1–7. http://arxiv.org/abs/1810.11363

Dulaimi, A., Al Busaltan, S., Mydin, M. A. O., Lu, D., Özkılıç, Y. O., Jaya, R. P., & Ameen, A. (2023). Innovative geopolymer-based cold asphalt emulsion mixture as eco-friendly material. *Scientific Reports*, *13*(1), 1–15. https://doi.org/10.1038/s41598-023-44630-5

Eleyedath, A., & Swamy, A. K. (2022). Prediction of dynamic modulus of asphalt concrete using hybrid machine learning technique. *International Journal of Pavement Engineering*, *23*(6), 2083–2098. https://doi.org/10.1080/10298436.2020.1841191

Elmuna, E. A. F., Chamidy, T., & Nugroho, F. (2023). Optimization of the Random Forest Method Using Principal Component Analysis to Predict House Prices. *International Journal of Advances in Data and Information Systems, 4*(2), 155–166. https://doi.org/10.25008/ijadis.v4i2.1290

Feng Zhang, C. H. (2015). Preparation and properties of high viscosity modified asphalt.

Polymer Composites, *38*(5), 936–946.

Friedman. (2001). Greedy function approximation: A gradient boosting machine. Annals of Statistics. *Annals of Statistics*, *29*, 1189–1232.

Golestani, B., Nam, B. H., Moghadas Nejad, F., & Fallah, S. (2015). Nanoclay application to asphalt concrete: Characterization of polymer and linear nanocomposite-modified asphalt binder and mixture. *Construction and Building Materials*, *91*, 32–38. https://doi.org/10.1016/j.conbuildmat.2015.05.019

Hamid, Abdulrahman, Hamed Alfaidi, Hassan Baaj, El-Hakim, and M. (2020). Evaluating fly ash-based geopolymers as a modifier for asphalt binders. *Advances in Materials Science and Engineering*, *1*.

Hussain, W. A. M., Abdulrasool, A. T., & Kadhim, Y. N. (2022). Using Nanoclay Hydrophilic Bentonite As a Filler To Enhance the Mechanical Properties of Asphalt. *Journal of Applied Engineering Science*, *20*(1), 300–304. https://doi.org/10.5937/jaes0-35111

Iam Palatnik de Sousa, M. M. B. R. V. and, & Silva, E. C. da. (2019). Local interpretable model-agnostic explanations for classification of lymph node metastases. *Sensors (Switzerland)*, *19*(13), 7–9. https://doi.org/10.3390/s19132969

Iskender, E. (2016). Evaluation of mechanical properties of nano-clay modified asphalt mixtures. *Measurement: Journal of the International Measurement Confederation*, *93*, 359–371. https://doi.org/10.1016/j.measurement.2016.07.045

Jamshidi, A., Hamzah, M. O., & Aman, M. Y. (2012). Effects of Sasobit® content on the rheological characteristics of unaged and aged asphalt binders at high and intermediate temperatures. *Materials Research*, *15*(4), 628–638. https://doi.org/10.1590/S1516-14392012005000083

Katanalp, B. Y., Tastan, M., & Ahmedzade, P. (2024). Recycling the electric arc furnace waste after geopolymerization in bitumen: experimental analyses and LCA study. *Materials and Structures/Materiaux et Constructions*, *57*(5), 1–24. https://doi.org/10.1617/s11527-024-02376-0

Khasawneh, M. A., Dernayka, S. D., & Chowdhury, S. R. (2023). Experimental characterization and environmental impact of different grades of CRM-modified asphalt binders. *Materials Research Proceedings*, *31*, 16–28. https://doi.org/10.21741/9781644902592-3

Lamontagne, J., Dumas, P., Mouillet, V., & Kister, J. (2001). Comparison by Fourier transform infrared (FTIR) spectroscopy of different ageing techniques: Application to road bitumens. *Fuel*, *80*(4), 483–488. https://doi.org/10.1016/S0016-2361(00)00121-6

Le, T. H., Nguyen, H. L., Pham, B. T., Nguyen, M. H., Pham, C. T., Nguyen, N. L., Le, T. T., & Ly, H. B. (2020). Artificial Intelligence-Based Model for the Prediction of Dynamic Modulus of Stone Mastic Asphalt. *Applied Sciences 2020, Vol. 10, Page 5242*, *10*(15), 5242. https://doi.org/10.3390/APP10155242

Lee, L. &. (2017). *A Unified Approach to Interpreting Model Predictions*.

Li, N., Zhan, H., Yu, X., Tang, W., Yu, H., & Dong, F. (2021). Research on the high temperature performance of asphalt pavement based on field cores with different rutting development levels. *Materials and Structures/Materiaux et Constructions*, *54*(2). https://doi.org/10.1617/s11527-021-01672-3

Li, T., Meng, Q., & Du, Q. (2020). Application of Random Effects to Explore the Gulf of Mexico Coastal Forest Dynamics in Relation to Meteorological Factors. *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, *13*, 5526–5535. https://doi.org/10.1109/JSTARS.2020.3024101

Li, Y., Yan, X., Guo, J., Wu, W., Shi, W., Xu, Q., & Ji, Z. (2023). Performance and Verification of High-Modulus Asphalt Modified by Styrene-Butadiene-Styrene Block Copolymer (SBS) and Rock Asphalt. *Coatings*, *13*(1). https://doi.org/10.3390/coatings13010038

Li, Z., Yu, X., Liang, Y., & Wu, S. (2021). Carbon nanomaterials for enhancing the thermal, physical and rheological properties of asphalt binders. *Materials*, *14*(10). https://doi.org/10.3390/ma14102585

Liu, J., Liu, F., Zheng, C., Zhou, D., & Wang, L. (2022). Optimizing asphalt mix design through predicting the rut depth of asphalt pavement using machine learning. *Construction and Building Materials*, *356*(February), 129211. https://doi.org/10.1016/j.conbuildmat.2022.129211

Liu, Y., Gong, W., Hu, X., & Gong, J. (2018). Forest type identification with random forest using Sentinel-1A, Sentinel-2A, multi-temporal Landsat-8 and DEM data. *Remote Sensing*, *10*(6), 1–25. https://doi.org/10.3390/rs10060946

Liu, Y., & Tang, X. (2023). *Study on the Effect of Anti-rutting Agent (NRP) on the Performance of Asphalt Mixture* (Issue Icsscer). Atlantis Press International BV. https://doi.org/10.2991/978-94-6463-312-2_17

Luo, X., Wang, H., Cao, S., Ling, J., Yang, S., & Zhang, Y. (2023). A hybrid approach for fatigue life prediction of in-service asphalt pavement. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, *381*(2254). https://doi.org/10.1098/rsta.2022.0174

Lv, C. X., An, S. Y., Qiao, B. J., & Wu, W. (2021). Time series analysis of hemorrhagic fever with renal syndrome in mainland China by using an XGBoost forecasting model. *BMC Infectious Diseases*, *21*(1), 1–13. https://doi.org/10.1186/s12879-021-06503-y

Miller, T. (2018). Explanation in Artificial Intelligence: Insights from the social sciences. *Artif. Intell*, *267*(1–38).

Molnar, C., König, G., Herbinger, J., Freiesleben, T., Dandl, S., Scholbeck, C. A., Casalicchio, G., Grosse-Wentrup, M., & Bischl, B. (2022). General Pitfalls of Model-Agnostic Interpretation Methods for Machine Learning Models. *Lecture Notes in Computer Science (Including Subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics), 39–68.*

Muliauwan, H. N., Prayogo, D., Gaby, G., & Harsono, K. (2020). Prediction of Concrete Compressive Strength Using Artificial Intelligence Methods. *Journal of Physics:*

Conference Series, *1625*(1). https://doi.org/10.1088/1742-6596/1625/1/012018

Olsson, E., Jelagin, D., & Partl, M. N. (2019). New discrete element framework for modelling asphalt compaction. *Road Materials and Pavement Design*, *20*(sup2), S604–S616. https://doi.org/10.1080/14680629.2019.1633750

Poursabzi-Sangdeh, F., Goldstein, D. G., & Hofman, J. M. (2021). Manipulating and measuring model interpretability. In *Conference on Human Factors in Computing Systems - Proceedings*. https://doi.org/10.1145/3411764.3445315

Ren, Y., Zhang, L., & Suganthan, P. N. (2016). Ensemble Classification and Regression-Recent Developments, Applications and Future Directions [Review Article]. *IEEE Computational Intelligence Magazine*, *11*(1), 41–53. https://doi.org/10.1109/MCI.2015.2471235

Rodríguez-Pérez, R., & Bajorath, J. (2020). Interpretation of machine learning models using shapley values: application to compound potency and multi-target activity predictions. *Journal of Computer-Aided Molecular Design*, *34*(10), 1013–1026. https://doi.org/10.1007/s10822-020-00314-0

Roja, K. L., Rehman, A., Ouederni, M., Krishnamoorthy, S. K., Abdala, A., & Masad, E. (2021). Influence of polymer structure and amount on microstructure and properties of polyethylene-modified asphalt binders. *Materials and Structures/Materiaux et Constructions*, *54*(2), 1–17. https://doi.org/10.1617/s11527-021-01683-0

Romeo, L., & Frontoni, E. (2022). A Unified Hierarchical XGBoost model for classifying priorities for COVID-19 vaccination campaign. *Pattern Recognition*, *121*, 108197. https://doi.org/10.1016/j.patcog.2021.108197

Sedthayutthaphong, N., Jitsangiam, P., Nikraz, H., Pra-Ai, S., Tantanee, S., & Nusit, K. (2021). The influence of a field-aged asphalt binder and aggregates on the skid resistance of recycled hot mix asphalt. *Sustainability (Switzerland)*, *13*(19), 1–16. https://doi.org/10.3390/su131910938

Shangxian Xie, Qiang Li, Pravat Kark, Fujie Zhou, J. S. Y. (2017). Lignin as renewable and superior asphalt binder modifier. *Acs Sustainable Chemistry & Engineering*, *5*(4).

Sulejmani, P., Said, S., Agardh, S., & Ahmed, A. (2019). Moisture Sensitivity of Asphalt Mixtures using Cycling Pore Pressure Conditioning. *Transportation Research*, 294–303. https://doi.org/10.1177/0361198118823496

Sun, Y., Wang, W., & Chen, J. (2019). Investigating impacts of warm-mix asphalt technologies and high reclaimed asphalt pavement binder content on rutting and fatigue performance of asphalt binder through MSCR and LAS tests. *Journal of Cleaner Production*, *219*, 879–893. https://doi.org/10.1016/j.jclepro.2019.02.131

Swathi, Y., & Challa, M. (2023). A Comparative Analysis of Explainable AI Techniques for Enhanced Model Interpretability. *Proceedings - 2023 3rd International Conference on Pervasive Computing and Social Networking, ICPCSN 2023*, 229–234. https://doi.org/10.1109/ICPCSN58827.2023.00043

Tiwari, R., Dubey, S., & Kumar, V. (2019). Interpretability machine learning models: A critical analysis of techniques and applications. *The Pharma Innovation*, *8*(2S), 25–28. https://doi.org/10.22271/tpi.2019.v8.i2sa.25245

Torlay, L., Perrone-Bertolotti, M., Thomas, E., & Baciu, M. (2017). Machine learning–XGBoost analysis of language networks to classify patients with epilepsy. *Brain Informatics, 4*(3), 159–169. https://doi.org/10.1007/s40708-017-0065-7

Toth, C., Petho, L., Rosta, S., & Primusz, P. (2023). Performance assessment of full depth asphalt pavements manufactured with high recycled asphalt pavement content. *Acta Technica Jaurinensis*, *16*(1), 18–26. https://doi.org/10.14513/actatechjaur.00688

Turbay, E., Martinez-Arguelles, G., Navarro-Donado, T., Sánchez-Cotte, E., Polo-Mendoza, R., & Covilla-Valera, E. (2022). Rheological Behaviour of WMA-Modified Asphalt Binders with Crumb Rubber. *Polymers*, *14*(19). https://doi.org/10.3390/polym14194148

Uwanuakwa, I. D., Ali, S. I. A., Hasan, M. R. M., Akpinar, P., Sani, A., & Shariff, K. A. (2020). Artificial intelligence prediction of rutting and fatigue parameters in modified asphalt binders. *Applied Sciences (Switzerland)*, *10*(21), 1–17. https://doi.org/10.3390/app10217764

Vaitkus, A., Žilioniene, D., Paulauskaite, S., Tuminiene, F., & Žiliute, L. (2011). Research and assessment of asphalt layers bonding. *Baltic Journal of Road and Bridge Engineering*, *6*(3), 210–218. https://doi.org/10.3846/bjrbe.2011.27

Van Dao, D., Nguyen, N. L., Ly, H. B., Pham, B. T., & Le, T. T. (2020). Cost-effective approaches based on machine learning to predict dynamic modulus of warm mix asphalt with high reclaimed asphalt pavement. *Materials*, *13*(15), 1–19. https://doi.org/10.3390/MA13153272

Wang, Chaohui Songyuan Tan, Qian Chen, Jiguo Han, L. S., & Fu, and Y. (2021). Dynamic Modulus Prediction of a High-Modulus Asphalt Mixture. *Advances in Civil Engineering*.

Wang, G., Wang, X., Yan, Z., Qin, L., & Gao, Z. (2020). Analysis of the Influence of Temperature Field on the Dynamic Modulus of Rubber Asphalt Pavement. *Frontiers in Materials*, *7*(October 2020), 1–11. https://doi.org/10.3389/fmats.2020.586457

Wang, X., Lu, T., Zhou, W., Ji, X., Lu, W., & Yang, J. (2022). Accelerated Discovery of Ternary Gold Alloy Materials with Low Resistivity via an Interpretable Machine Learning Strategy. *Chemistry - An Asian Journal*, *17*(22), 1–7. https://doi.org/10.1002/asia.202200771

Woszuk, A., Wróbel, M., & Franus, W. (2019). Influence of waste engine oil addition on the properties of zeolite-foamed asphalt. *Materials*, *12*(14). https://doi.org/10.3390/ma12142265

Wu, B., Luo, C., Pei, Z., Chen, C., Xia, J., & Xiao, P. (2021). Evaluation of the aging of styrene-butadiene-styrene modified asphalt binder with different polymer additives. *Materials*, *14*(19). https://doi.org/10.3390/ma14195715

Xu, B., Huang, J. Z., Williams, G., Li, M. J., & Ye, Y. (2012). Hybrid random forests: Advantages of mixed trees in classifying text data. *Lecture Notes in Computer Science (Including Subseries Lecture Notes in Artificial Intelligence and Lecture Notes in*

Bioinformatics), *7301 LNAI*(PART 1), 147–158. https://doi.org/10.1007/978-3-642-30217-6_13

Yang, Shirui Sun, Hongfu Mi, Wenhe Wang, J. L. and Z. Y. K. (2024). Interpretable Feedforward Neural Network and XGBoost-Based Algorithms to Predict CO2 Solubility in Ionic Liquids. *Industrial & Engineering Chemistry Research*, *63*(18).

Zhan, X. L. (2013). Prediction of Dynamic Modulus of Asphalt Mixture Based on Viscoelastic Properties of Asphalt Mortar. *Advanced Materials Research*, *651*, 419–423.

Zhang, C., Wang, H., You, Z., Gao, J., & Irfan, M. (2019). Performance test on Styrene-Butadiene-Styrene (SBS) modified asphalt based on the different evaluation methods. *Applied Sciences (Switzerland)*, *9*(3), 1–11. https://doi.org/10.3390/app9030467

Zhang, F., Wang, L., Li, C., & Xing, Y. (2020). Predict the phase angle master curve and study the viscoelastic properties of warm mix crumb rubber-modified asphalt mixture. *Materials*, *13*(21), 1–26. https://doi.org/10.3390/ma13215051

Zhang, G., Hui, G., Yang, A., & Zhao, Z. (2021). A simple and effective approach to quantitatively characterize structural complexity. *Scientific Reports*, *11*(1), 1–11. https://doi.org/10.1038/s41598-020-79334-7

Zhang, X., Han, C., Yang, J., Xu, X., & Zhang, F. (2021). Evaluating the rheological properties of high-modulus asphalt binders modified with rubber polymer composite modifier. *Materials*, *14*(24). https://doi.org/10.3390/ma14247727

Zhang, Y., Ma, J., Liang, S., Li, X., & Li, M. (2020). An evaluation of eight machine learning regression algorithms for forest aboveground biomass estimation from multiple satellite data products. *Remote Sensing*, *12*(24), 1–26. https://doi.org/10.3390/rs12244015

Zhou, H. Y., Dou, H. B., & Chen, X. H. (2021). Rheological properties of graphene/polyethylene composite modified asphalt binder. *Materials*, *14*(14), 1–15. https://doi.org/10.3390/ma14143986

APPENDICES

Appendix A

Supplementary LIME illustrations

The figure below shows the result of LME for the three models used. Here is the finding of the remain six instances as said in chapter four which were presented in this section.

Figure 19

LIME of storage modulus for CatBoost

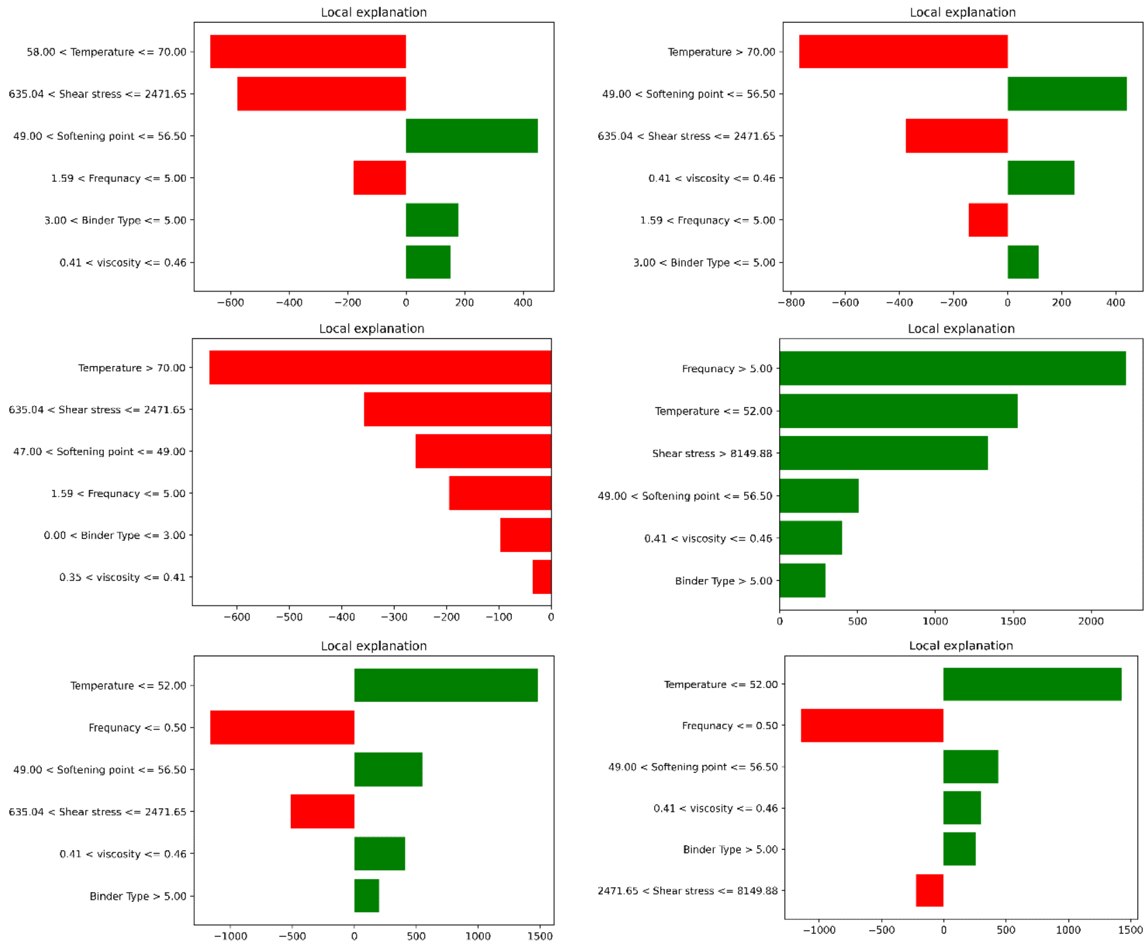


Figure 20

LIME of storage modulus for Random Forest

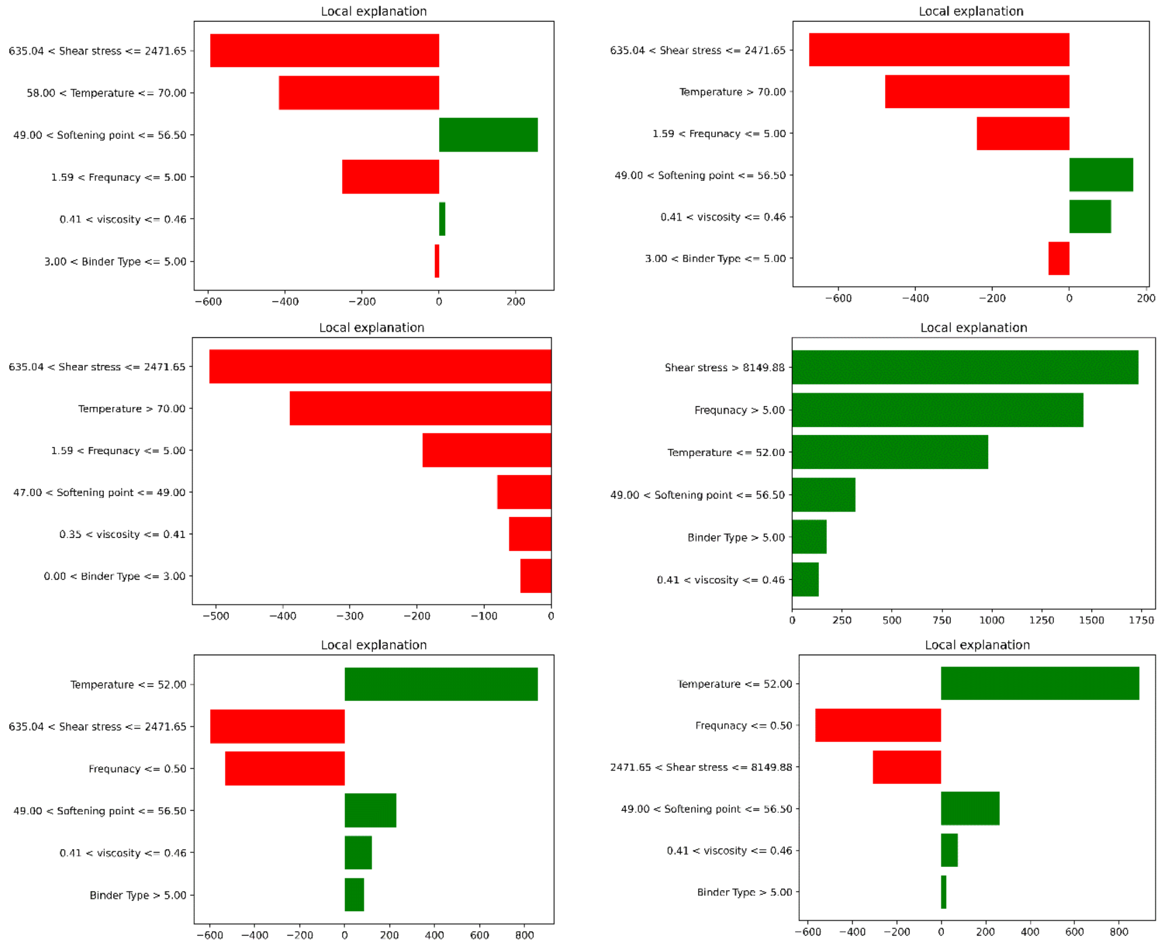


Figure 21

LIME of storage modulus for XGBoost

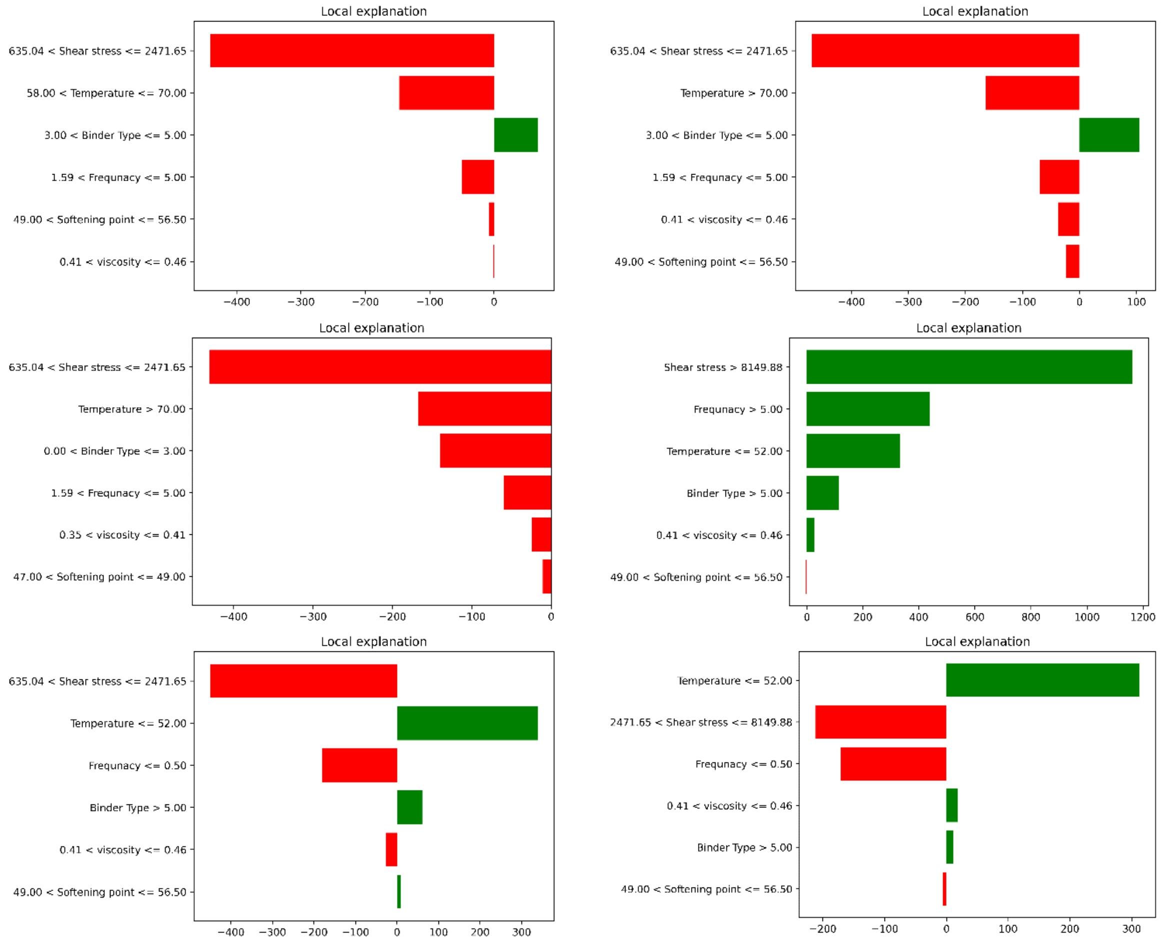


Figure 22

LIME of loss modulus for CatBoost

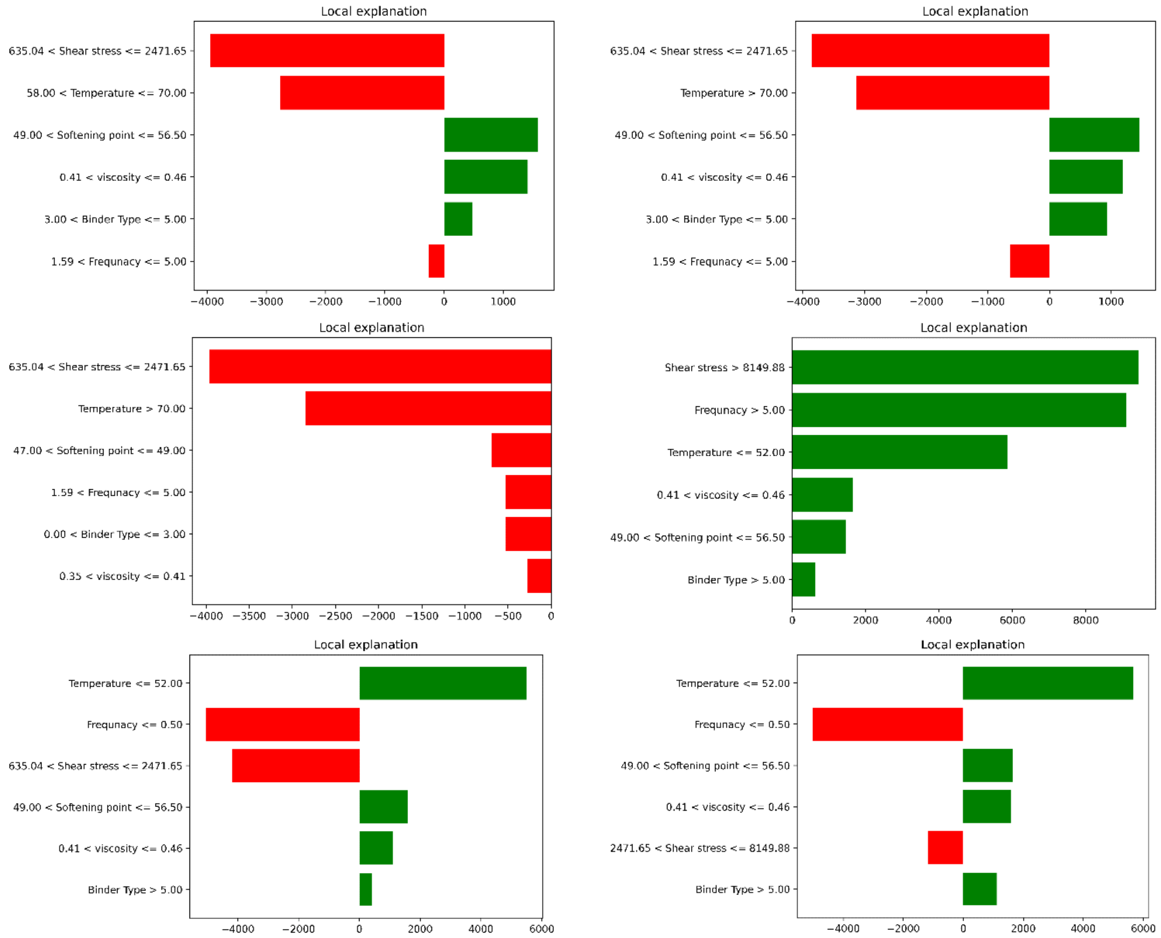


Figure 23

LIME of loss modulus for Random Forest

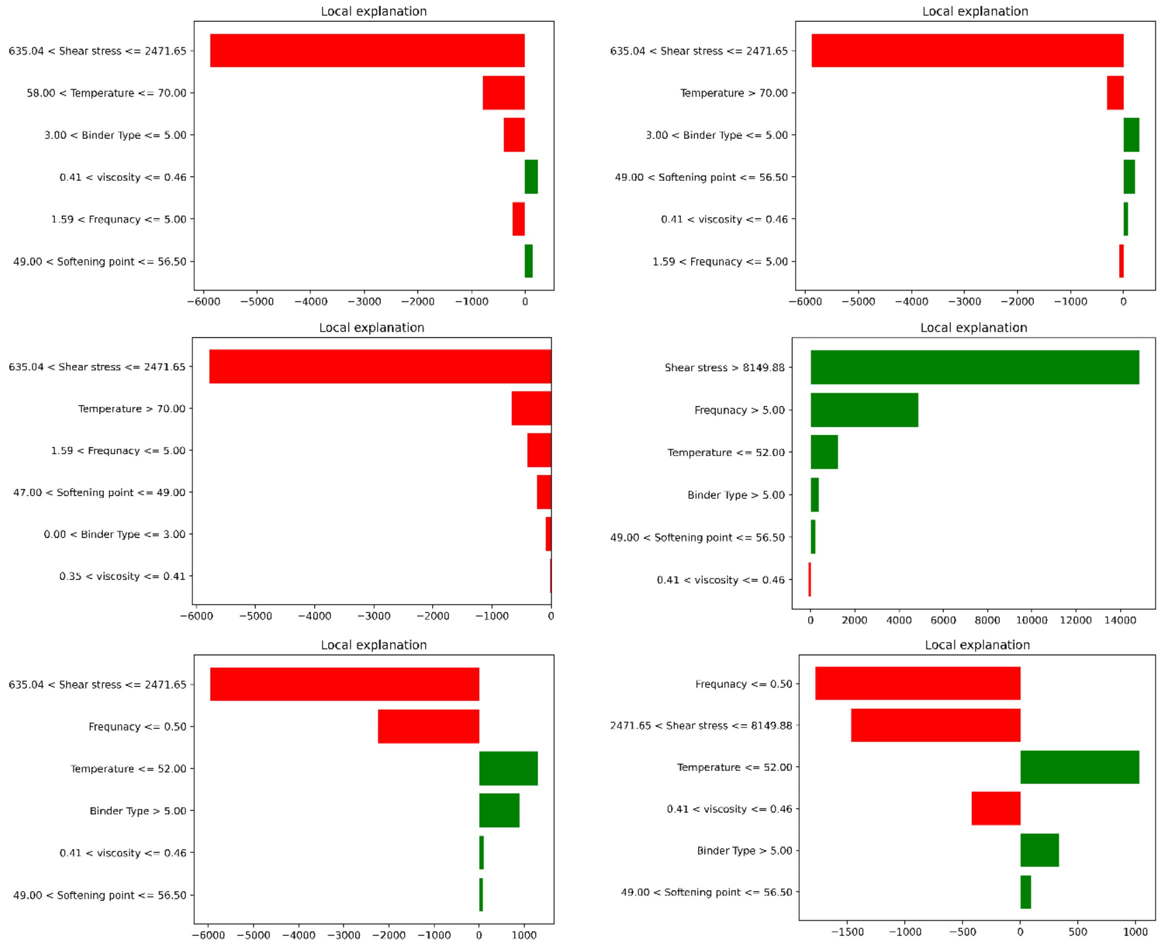
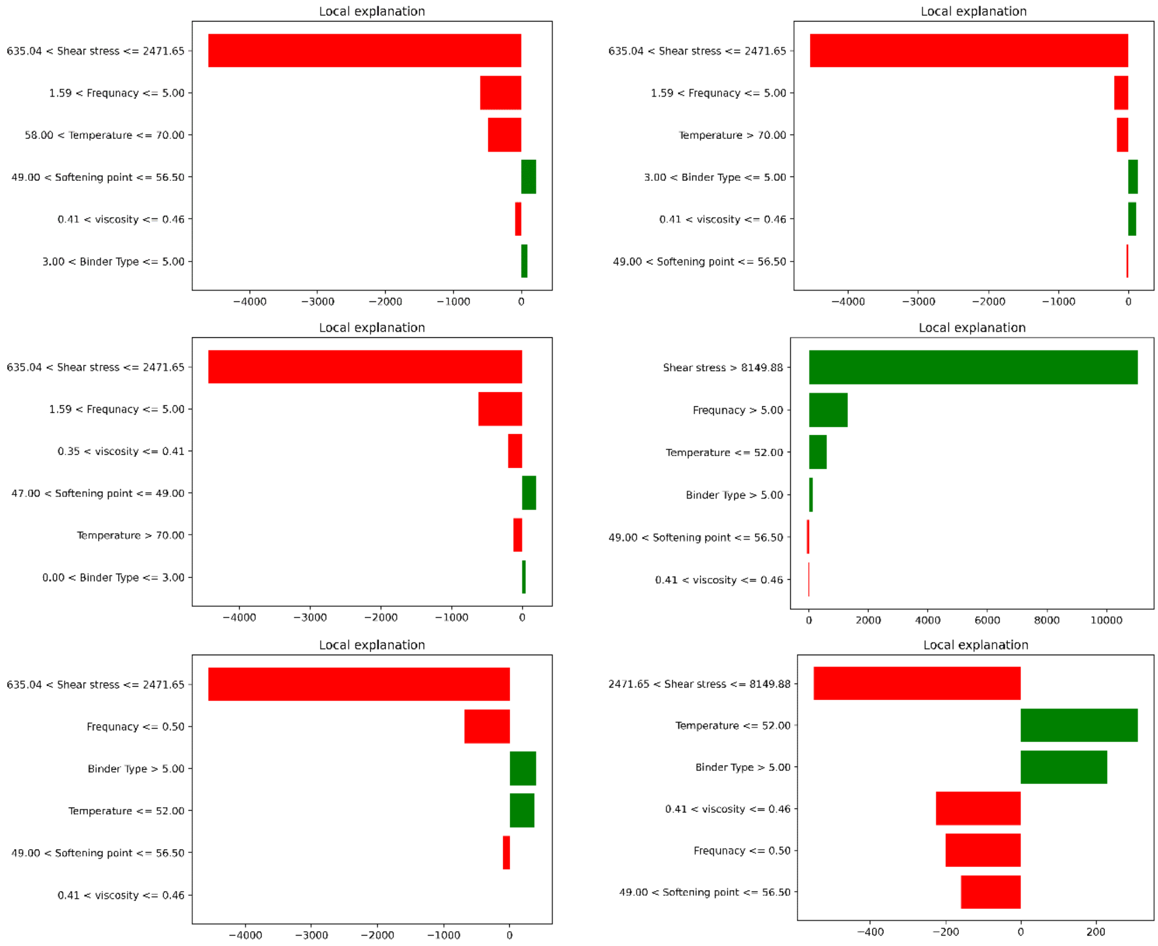


Figure 24

LIME of loss modulus for XGBoost



Supplementary ICI illustrations

Figure 25

ICI Values of different models for Loss Modulus prediction

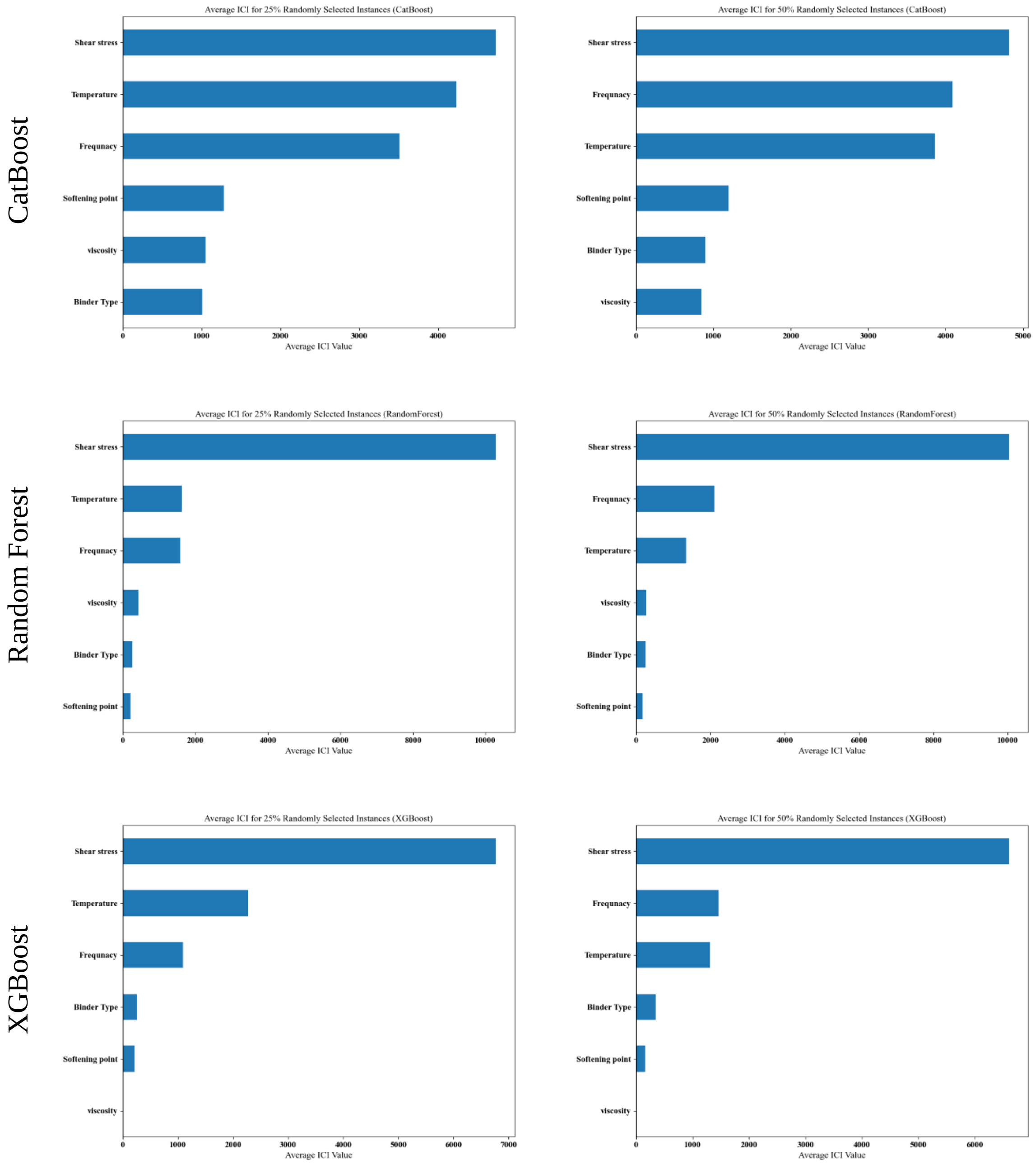
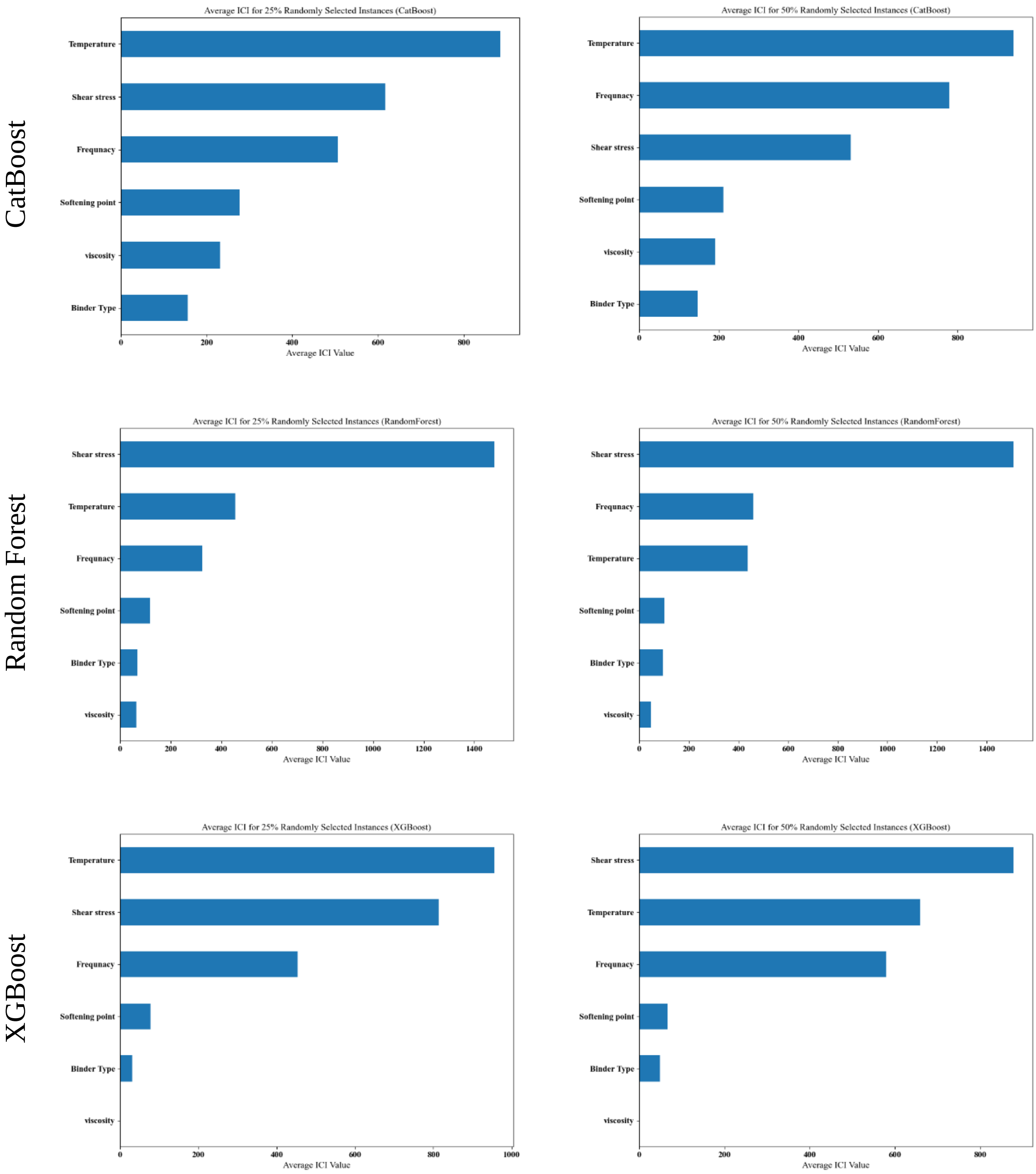


Figure 26

ICI Values of different models for Storage Modulus prediction



Appendix B

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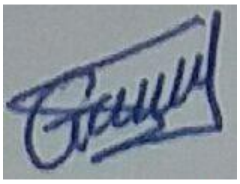


Assist. Prof. Dr. Gebre Gelete Kebede

Supervisor

Appendix C

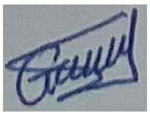
Ethical approval letter

Reference: Lyce Ndolo Umba – 20225164

I would like to inform you that the above candidate is one of our postgraduate students in Civil Engineering Department. She is taking thesis under my supervision and the thesis title is: **"Prediction of high-temperature performance of geopolymer modified asphalt binder using machine learning and model interpretation approach".** Since the researcher(s) did not collect primary data from humans, animals or plants, this project does not need to go through the ethics committee. Please do not hesitate to contact me if you have any further queries or questions.

Thank you very much indeed.

Best Regards.



Assist. Prof. Dr. Gebre Gelete Kebede