A MULTIMODEL REGRESSION APPROACH TO FORECASTING MINERAL HARDNESS FROM CHEMICAL AND PHYSICAL FEATURE

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ABSTRACT

Mineral hardness and density serve as fundamental physical characteristics in fields such as geology, mining, and material science, where they are widely used for mineral identification and classification. Conventionally, hardness was evaluated using the Mohs scale through manual scratch testing, in which minerals were compared against standard reference specimens. This process typically demanded laboratory facilities, domain expertise, and considerable time to achieve reliable results. Moreover, it was often labor-intensive and prone to inconsistencies arising from human error and varying experimental conditions. To overcome these challenges, the proposed work presents a Machine Learning driven multimodel regression framework designed to estimate mineral hardness and specific gravity based on their chemical and physical attributes. The system is developed as a web-based application using the Django framework, enabling an interactive and accessible platform. Multiple regression techniques are employed to enhance predictive accuracy, including CatBoost Regressor (CBR), AdaBoost Regressor (ABR), Random Forest Regressor (RFR), and a hybrid ML and Deep Learning (DL) model as Greedy Tab Transformer (GTT). These models learn the relationships between mineral features and target variables to generate accurate predictions for Mohs hardness and specific gravity. Experimental results indicate that the GTT model achieves superior predictive performance compared to the other approaches. In addition to prediction, the system incorporates functionalities such as model training, comparative analysis of algorithms, and prediction modules for evaluating mineral properties. By combining ML techniques with a web-based interface, the system provides a more efficient, scalable, and reliable alternative to traditional manual testing methods for mineral property prediction.

1. INTRODUCTION

The identification and characterization of rock types, as illustrated in Fig. 1, play a crucial role in various domains of earth sciences and mining engineering. Accurate classification is essential throughout different stages, from initial design and feasibility analysis to the execution of mining operations. It significantly influences the selection of mining methods, equipment planning, and overall operational safety. Effective rock characterization ensures efficient resource utilization while reducing potential risks during extraction processes. Conventional approaches for determining rock types primarily rely on laboratory testing, field investigations, and expert interpretation. Although these methods are widely adopted, they are often time-consuming, labor-intensive, and require specialized expertise. Additionally, variations in geological conditions and subjective judgment may lead to inconsistencies or inaccuracies in classification. To overcome these limitations, statistical and computational methods have been introduced to estimate rock types using previously analyzed rock parameters. In recent years, data mining has emerged as a powerful approach for analyzing complex geotechnical datasets. It focuses on extracting meaningful and actionable information from large volumes of structured and unstructured data. Unlike traditional statistical techniques, data mining utilizes advanced algorithms to uncover hidden patterns, correlations, and non-linear relationships within datasets, making it highly effective for solving complex engineering problems [1].

A significant body of research has focused on predicting rock properties that are difficult, costly, or time-intensive to measure through conventional experiments. Most studies emphasize the estimation of mechanical properties such as elastic modulus and strength parameters. It has been observed that data mining techniques often outperform traditional empirical and statistical methods in terms of prediction accuracy and robustness [2,3]. However, the application of these approaches is sometimes limited due to the requirement of domain-specific expertise and high-quality datasets. Several studies have proposed models for predicting key geomechanical parameters such as deformation modulus, friction angle, cohesion, and strength characteristics using various data mining techniques.

Fig. 1.1: Minerals of hardness

Methods including multiple regression, artificial neural networks, and support vector machines have been widely applied for estimating properties like uniaxial compressive strength and modulus of elasticity. Among these approaches, support vector-based methods have demonstrated superior predictive performance in certain cases, highlighting their effectiveness in modeling complex relationships within rock data [4,5].

2. LITERATURE SURVEY

Bassi, et al. [6] proposed an AI-based model that can simultaneously predict the hardness and phase fraction percentages of micro-alloyed steel with a predefined chemical composition and thermomechanical processing conditions. Specifically, the model uses a feed-forward neural network enhanced by the ensemble method. The model has been trained on experimental data derived from continuous cooling transformation (CCT) diagrams of 39 different steels. The inputs to the model include a cooling profile defined by a set of time-temperature values and the chemical composition of the steel. Sensitivity analysis was performed on the validated model to understand the impact of key input variables, including individual alloys and the thermomechanical processing conditions. This analysis, which measures the variability in output in response to changes in a specific input variable, showed excellent agreement with experimental data and the trends in the literature. Paturi, et al. [7] evaluated the predictive capabilities of various ML (ML) algorithms for estimating the hardness of AlCoCrCuFeNi high-entropy alloys (HEAs) based on their compositional variables. Among the ML methods explored, a backpropagation neural network (BPNN) model with a sigmoid activation function exhibited superior predictive accuracy compared to other algorithms. The BPNN model achieved excellent correlation coefficients (R^2) of 99.54% and 96.39% for training (116 datasets) and cross-validation (39 datasets), respectively. Testing of the BPNN model on an independent dataset (14 alloys) further confirmed its high predictive reliability. Additionally, the developed BPNN model facilitated a comprehensive analysis of the individual effects of alloying elements on hardness, providing valuable metallurgical insights. This comparative evaluation highlights the potential of BPNN as an effective predictive tool for material scientists aiming to understand composition–property relationships in HEAs. Rodríguez-Rosales, et al. [8] evaluated the effect of temperature and time austempering on microstructural characteristics and hardness of ductile iron, validating the results by means of a statistical method for hardness prediction. Ductile iron was subjected to austenitization at 950 °C for 120 min and then to austempering heat treatment in a salt bath at temperatures of 290, 320, 350 and 380 °C for 30, 60, 90 and 120 min. By increasing austempering temperature, a higher content of carbon-rich austenite was obtained, and the morphology of the thin acicular ferrite needles produced at 290 °C turned completely feathery at 350 and 380 °C. A thickening of acicular ferrite needles was also observed as austempering time increased. An inversely proportional behavior of hardness values was thus obtained, which was validated through data analysis, statistical tools and a regression model taking temperature and time austempering as input variables and hardness as the output variable, which achieved a correlation among variables of about 97%.

Liu, et al. [9] proposed a machine-learning approach to predict extraterrestrial rock hardness using morphological features. A custom dataset of 1496 rock images, including granite, limestone, basalt, and sandstone, was created. Ten features, such as roundness, elongation, convexity, and Lab color values, were extracted for prediction. A foundational model combining Random Forest (RF) and Support Vector Regression (SVR) was trained through cross-validation. The output of this model was used as the input for a meta-model, undergoing linear fitting to predict Mohs hardness, forming the Meta-Random Forest and Support Vector Regression (MRFSVR) model. The model achieved an R^2 of 0.8219, an MSE of 0.2514, and a mean absolute error of 0.2431 during validation. Meteorite samples were used to validate the MRFSVR model's predictions. The model is used to predict the hardness distribution of extraterrestrial rocks using images from the Tianwen-1 Mars Rover Navigation and Terrain Camera (NaTeCam) and a simulated lunar rock dataset from an open-source website. Bermanec, et al. [10] described the survey of the average Mohs hardness of minerals throughout Earth's history reveals a significant and systematic decrease from >6 in presolar grains to ~5 for Archean lithologies to <4 for Phanerozoic minerals. Two primary factors contribute to this temporal decrease in the average Mohs hardness. First, selective losses of softer minerals throughout billions of years of near-surface processing lead to preservational biases in the mineral record. Second, changes in the processes of mineral formation play a significant role because more ancient refractory stellar phases and primary igneous minerals of the Hadean/Archean Eon are intrinsically harder than more recently weathered products, especially following the Paleoproterozoic Great Oxidation Event and the production of Phanerozoic biominerals. Dubey, et al. [11] involved several gemstones: amethyst, aquamarine beryl, bloodstone citrine, diopside, and enstatite. Their hardness is determined through a correlation utilizing the spectral intensity ratio of the ionic to atomic spectral lines of an identified element in the LIB spectrum. The result of the relative hardness obtained from the LIBS analysis is in good agreement with the hardness measured from Mohs's scale of hardness, a popular qualitative method to determine hardness. In this work, a linear relationship has been established between the Mohs's hardness and the plasma excitation temperature. Thus, the hardness of the gemstones can be determined with the help of plasma excitation temperature. Moreover, the analysis of trace elements in LIB spectral data reveals that a particular element is responsible for the colors of gemstones. Therefore, the relative concentration of constituents is calculated for all gemstones and compared. Principal component analysis (PCA) is successfully applied to all gemstone spectra for rapid classification and discrimination based on their variable elemental concentrations and respective hardness.

Castillo, et al. [12] conducted a comprehensive physical, chemical, mineralogical, and toxicological characterization of ten active and inactive tailings samples from the Arequipa region in southern Peru. Particle size distribution analysis, inductively coupled plasma atomic emission spectroscopy (ICP-AES), scanning electron microscopy with energy-dispersive spectroscopy (SEM-EDS), and the Toxicity Characteristic Leaching Procedure (TCLP) followed by ICP-MS were employed. The results revealed variable particle size distributions, with the sample of Secocha exhibiting the finest granulometry. Chemically, 8 out of 10 samples exhibited concentrations of at least two metals surpassing the Peruvian Environmental Quality Standards (EQS) for soils with values reaching >6000 mg/kg of arsenic (Paraiso), 193.1 mg/kg of mercury (Mollehuaca), and 2309 mg/kg of zinc (Paraiso). Mineralogical analysis revealed the presence of sulfides such as arsenopyrite, cinnabar, galena, and sphalerite, along with uraninite in the Otapara sample. In the TCLP tests, 5 out of 10 samples released at least two metals exceeding the environmental standards on water quality, with concentrations up to 0.401 mg/L for mercury (Paraiso), 0.590 mg/L for lead (Paraiso), and 9.286 mg/L for zinc (Kiowa Cobre). Bombac, et al. [13] developed methodology for determining the physical properties of mineral fibers prepared from different input mixtures under the same spinning wheel conditions is described and discussed. Energy dispersive X-ray fluorescence spectroscopy was combined with simultaneous thermal analysis and thermogravimetry to study the mineralogical composition and typical melting and crystallization temperatures. The mechanical properties measured with nanoindentation were related to the mineralogical properties and the results obtained agree with the literature. The developed methodology shows reliable performance and demonstrates the ability to study the mechanical properties of mineral fibres, their mineralogical composition, and thermal properties. The presented experimental methodology opens up the possibility of researching the mechanical properties of mineral fibers for the purpose of defining production recipes in the field of mineral thermal insulation materials. El-Beltagi, et al. [14] aimed the study was to evaluate the phytochemical, mineral, extraction yield, total phenolic, total flavonoids, antioxidant, and antibacterial activity of several peel fruits, including Citrus sinensis (orange) and Punica granatum (pomegranate). The results revealed that pomegranate peel powder contains the highest amounts of ash, fiber, total carbohydrates, Ca, Fe, Mg, and Cu, while orange peel contains the highest amounts of moisture, protein, crude fat, P, and K. Furthermore, the aqueous and methanolic pomegranate peel extracts yielded higher total phenolic and total flavonoids than the orange peel extract. The identification and quantification of polyphenol compounds belonging to different classes, such as tannins, phenolic acids, and flavonoids in pomegranate peel and flavonoid compounds in orange peel were performed using UPLC-MS/MS. In addition, GC-MS analysis of orange peel essential oil discovered that the predominant compound is D-Limonene (95.7%).

3. PROPOSED SYSTEM

The proposed system integrates data processing, model training, and deployment within a unified pipeline to enable efficient prediction of target variables. Initially, raw data from the dataset is processed using an ML manager module, where relevant features and targets are extracted and prepared for further analysis. The processed data is then divided into training and testing subsets to ensure reliable model evaluation. Multiple existing models such as CBR, ABR, RFR approaches are trained alongside the proposed GTT hybrid model to enable comparative analysis. The trained models generate predictions, which are evaluated using performance metrics such as MAE, MSE, RMSE, and R^2 score is illustrated in Fig. 4.1. The system is deployed through a Django web-based interface, where the backend handles model execution and the frontend provide visualization, training insights, and prediction functionalities for different user roles. The architecture ensures scalability, modularity, and efficient interaction between data processing, model training, and user-level operations.

Data Acquisition and Preprocessing: The system begins by loading the dataset and passing it through a management module responsible for extracting relevant features and target variables. Data preprocessing techniques such as encoding and cleaning are applied to ensure consistency and usability. This step transforms raw data into a structured format suitable for ML models.

Feature and Target Separation: After preprocessing, the dataset is divided into input features and corresponding target variables. Feature engineering techniques may be applied to improve data representation and model performance. This step ensures that the models receive well-defined inputs for learning patterns effectively.

Train-Test Splitting: The processed dataset is split into training and testing subsets to evaluate model generalization. The training data is used to build the models, while the testing data is reserved for performance validation. This helps prevent overfitting and ensures reliable evaluation of model accuracy.

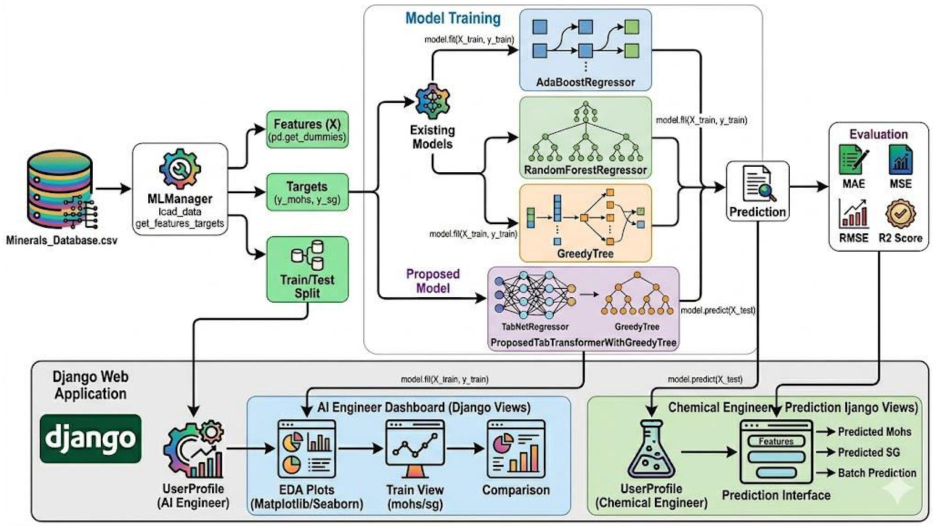


Fig. 4.1: Proposed system architecture.

Model Training and Development: In this stage, multiple models including AdaBoost Regressor, Random Forest Regressor, Decision Tree-based models, and the proposed TabNet-based model are trained using the training dataset. Each model learns patterns and relationships within the data to make predictions. The inclusion of multiple models enables comparative performance analysis.

Prediction and Evaluation: The trained models generate predictions on unseen test data. These predictions are evaluated using standard regression metrics such as MAE, MSE, RMSE, and R^2 score. This step helps in identifying the most effective model based on performance and accuracy.

Deployment and User Interaction: The final system is deployed through a web application interface, enabling interaction for different user roles. Engineers can perform model training, visualization, and comparison, while end-users can input data and obtain predictions. This ensures practical usability and real-time decision support.

3.1 GTT MODEL

GTT is an advanced ML model designed for handling tabular datasets by combining transformer-based learning with greedy feature selection techniques. It is particularly effective for datasets that contain multiple numerical and categorical attributes. The model learns complex relationships between different features by using attention mechanisms that allow it to focus on the most relevant information in the dataset. This approach helps improve prediction accuracy when compared to traditional regression algorithms. The working principle of GTT is based on the transformer architecture, where the model processes input features through multiple attention layers. These layers analyze the relationships between different attributes in the dataset and assign importance to the most relevant features. The greedy strategy further improves the model by selecting the most informative features step by step, allowing the model to concentrate on attributes that contribute the most to prediction performance as shown in Fig. 3.

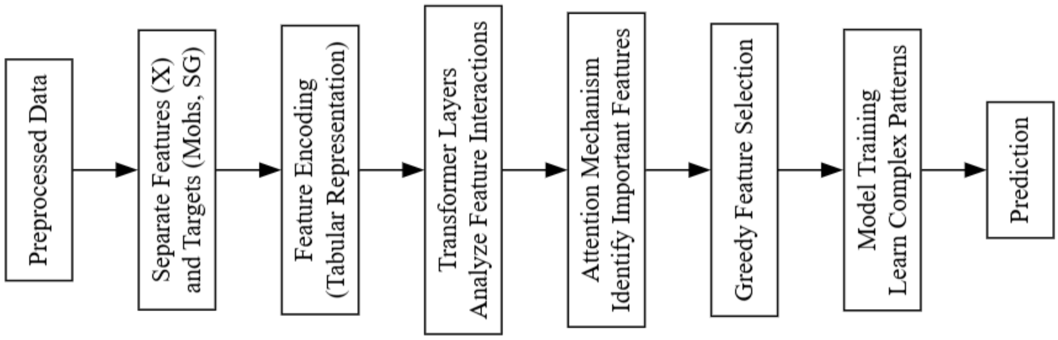


Fig. 3: Internal working of GTT model.

Input Dataset Preparation: The mineral dataset containing various chemical and physical attributes is used as the input for the GTT model. These attributes include properties such as refractive index, crystal structure, optical properties, mineral composition, and other related features. Before model training, the dataset passes through the preprocessing stage to ensure that the data is clean, structured, and suitable for ML analysis.

Feature and Target Separation: After preprocessing, the dataset is divided into input features and target variables. The mineral attributes are treated as input features, while Mohs Hardness and Specific Gravity are considered the target variables. This separation enables the model to learn the relationships between the mineral properties and their corresponding hardness and density values.

Feature Encoding and Representation: In this step, the input features are transformed into a numerical representation that can be processed by the model. The dataset is organized in a tabular format so that each mineral feature can be analyzed effectively. This representation allows the model to understand the relationships between different attributes.

Transformer-Based Feature Interaction: The GTT model uses transformer layers to analyze interactions between different input features. Through attention mechanisms, the model evaluates the importance of each feature and identifies how different attributes influence the prediction of hardness and specific gravity. This step helps the model capture complex patterns present in the dataset.

Greedy Feature Selection Process: During the training stage, the greedy strategy is applied to select the most informative features. The model iteratively evaluates feature importance and focuses on the attributes that contribute most to prediction accuracy. This process improves the efficiency of the model by reducing the influence of less relevant features.

Model Training and Learning Patterns: Once the important features are identified, the model is trained to learn the relationships between the selected features and the target variables. The transformer-based learning mechanism allows the model to understand complex dependencies within the dataset and improve prediction capability.

Model Evaluation and Prediction: After training is completed, the model is evaluated using test data to measure its prediction performance. The predicted values are compared with the actual values of Mohs hardness and specific gravity. Once validated, the trained GTT model is used in the system to generate predictions for new mineral input data.

3. RESULTS DESCRIPTION

Fig. 4 depicts the scatter plot representing the relationship between actual and predicted values of the Mohs hardness attribute using the GTT model. The visualization demonstrates the model's predictive performance by comparing observed hardness values against the corresponding estimated outputs. The alignment of data points along the diagonal reference line indicates a strong correlation and high prediction accuracy achieved by the model. The figure reflects the capability of the transformer-based approach to effectively learn complex patterns from tabular mineral data. It also highlights the consistency of predictions across a wide range of hardness values, suggesting minimal deviation and reduced prediction error. The distribution of points signifies the robustness of the model in handling both lower and higher hardness ranges.

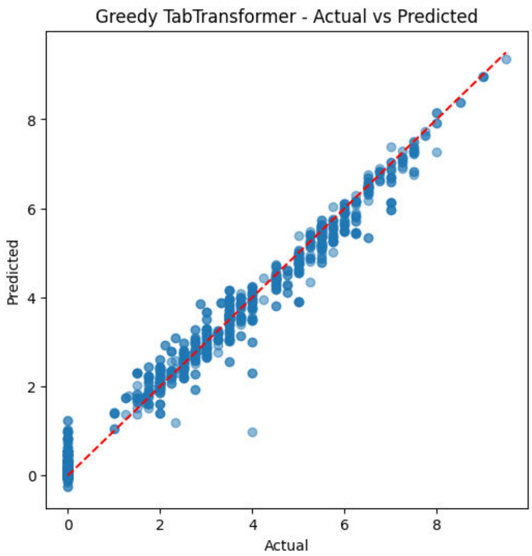


Fig. 4: Scatter plot of mohs hardness target attribute of GTT Model

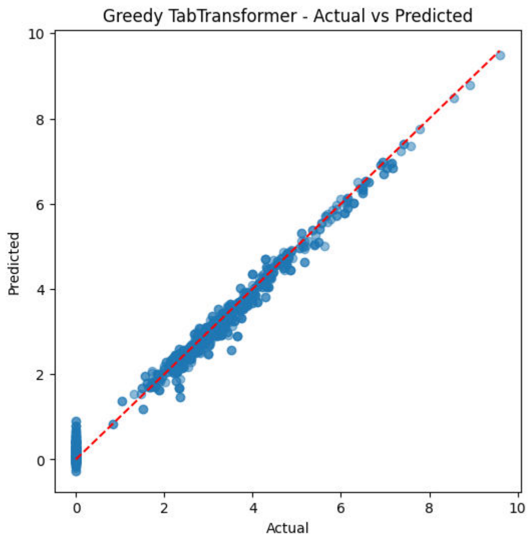
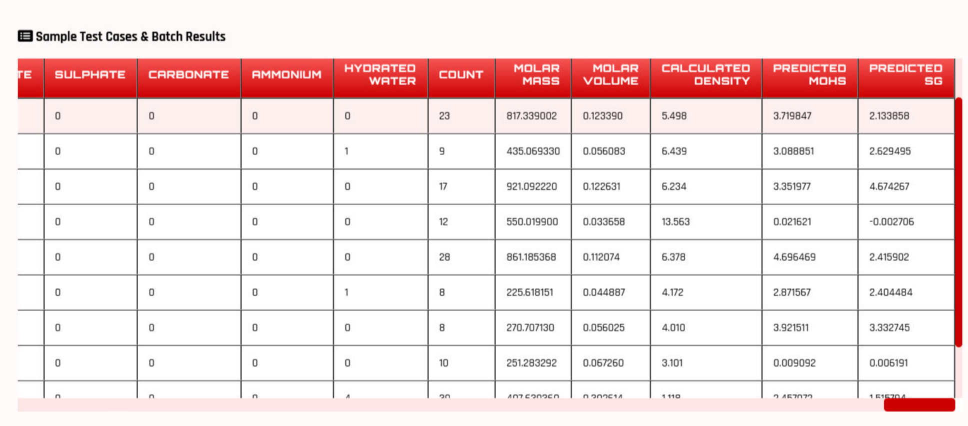


Fig. 5: Scatter plots of specific gravity target attribute of GTT Model

Fig. 5 illustrates the scatter plot comparing actual and predicted values of the specific gravity attribute using the GTT model. The figure demonstrates the effectiveness of the model in capturing the underlying relationship between mineral properties and their corresponding density-related characteristics. The close clustering of points around the diagonal reference line indicates a high degree of prediction accuracy and strong model generalization. It reflects the ability of the model to process complex feature interactions and generate precise regression outputs. The distribution pattern shows that the prediction error remains minimal across different value ranges, confirming the stability of the model. Additionally, the visualization emphasizes the suitability of transformer-based architectures for continuous value prediction tasks in geological datasets.


Sample Test Cases & Batch Results

TE	SULPHATE	CARBONATE	AMMONIUM	HYDRATED WATER	COUNT	MOLAR MASS	MOLAR VOLUME	CALCULATED DENSITY	PREDICTED MOHS	PREDICTED SG
	0	0	0	0	23	817.339002	0.123390	5.498	3.719847	2.133858
	0	0	0	1	9	435.069330	0.056083	6.439	3.088851	2.629495
	0	0	0	0	17	921.092220	0.122631	6.234	3.351977	4.674267
	0	0	0	0	12	550.019900	0.033658	13.563	0.021621	-0.002706
	0	0	0	0	28	861.185368	0.112074	6.378	4.696469	2.415902
	0	0	0	1	8	225.618151	0.044887	4.172	2.871567	2.404484
	0	0	0	0	8	270.707130	0.056025	4.010	3.921511	3.332745
	0	0	0	0	10	251.283292	0.067260	3.101	0.009092	0.006191

Fig. 6: Prediction results from test csv file.

Fig. 6 shows the Prediction Results interface, where the system displays the predicted outputs for the uploaded mineral dataset. The page presents a tabular view of input features such as Name, Chemical Composition (Iron, Silicon, etc.), Crystal Structure, Optical Properties, Refractive Index, along with the model-generated predictions for Mohs hardness and specific gravity appended to the dataset. Users can verify individual predictions directly and download the complete results in CSV format for further analysis. This screen allows seamless evaluation of batch prediction results and supports validation of the models' performance on unseen mineral samples

The table 1 presents a comparative analysis of four regression models CBR, ABR, RFR, and GTT for predicting Mohs hardness. Among these models, the GTT demonstrates superior performance, achieving the lowest error values with an MAE of 0.0459, MSE of 0.0205, and RMSE of 0.1432. It also records the highest R^2 score of 0.9908, indicating an excellent fit and very high predictive accuracy. RFR and CBR show moderate performance, with RMSE values of 0.5780 and 0.5854, respectively, and R^2 scores around 0.85, reflecting reasonable prediction accuracy. ABR exhibits the weakest performance, with the highest MAE (0.2722), MSE (0.5084), and RMSE (0.7130), along with the lowest R^2 (0.7713). These results confirm that GTT provides the most precise and reliable predictions for Mohs hardness among all evaluated models, highlighting its effectiveness in capturing complex relationships between chemical and physical mineral features.

Table. 1: Performance comparison of mohs hardness using various models

Algorithm	MAE	MSE	RMSE	R^2 Score
CBR Model	0.1895	0.3427	0.5854	0.8458
ABR Model	0.2722	0.5084	0.7130	0.7713
RFR Model	0.1773	0.3340	0.5780	0.8497

GTT Model	0.0459	0.0205	0.1432	0.9908

The table 2 presents a performance comparison of four regression models CBR, ABR, RFR, and GTT for predicting Specific Gravity. Among these models, the GTT achieves the best performance, with the lowest errors: MAE of 0.0290, MSE of 0.0075, and RMSE of 0.0869. It also records the highest R^2 score of 0.9947, reflecting excellent prediction accuracy and model fit. RFR and CBR demonstrate moderate performance, with RMSE values of 0.4123 and 0.4549, and R^2 scores of 0.8813 and 0.8555, respectively, indicating reasonable predictive capability. ABR performs the weakest, showing the highest error values and the lowest R^2 score of 0.7805. Overall, these results confirm that GTT provides the most precise and reliable predictions for Specific Gravity, effectively capturing complex relationships between the chemical and physical properties of minerals.

Table. 2: Performance comparison of specific gravity using various models

Algorithm	MAE	MSE	RMSE	R^2 Score
CBR Model	0.1320	0.2069	0.4549	0.8555
ABR Model	0.1764	0.3144	0.5607	0.7805
RFR Model	0.1136	0.1700	0.4123	0.8813
GTT Model	0.0290	0.0075	0.0869	0.9947

5. CONCLUSION

This study presents a multimodel regression framework designed to predict Mohs hardness and specific gravity of minerals using a combination of chemical and physical attributes. The system incorporates multiple ML models, including CBR, ABR, RFR, and GTT, along with enhanced feature representation through Tabnet Transformer. Among the implemented models, GTT demonstrates superior performance by achieving lower MAE, MSE, and RMSE values, along with higher R^2 scores compared to other approaches. The feature representation generated through TT effectively captures complex interactions among mineral characteristics, while the GT component contributes to improved decision boundaries, enhancing both interpretability and prediction stability. The integration of multiple models within a unified framework ensures consistent and reliable predictive outcomes. Experimental results indicate that the proposed system outperforms conventional methods that rely on manual testing procedures for determining mineral properties. The developed web-based framework provides a scalable and efficient solution suitable for real-world applications such as mineral classification, quality evaluation, and geological analysis. Furthermore, the approach reduces dependence on time-consuming laboratory experiments and supports faster, data-driven decision-making in both scientific and industrial environments.

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