J Inno Sci Eng, 2026, 10(1):46-64

DOI:https://doi.org/10.38088/jise.1769011

Research Article

Quantitative Prediction of Ti6Al4V Tribological Behavior Using Advanced Machine Learning Regression with Feature Engineering and Ensemble Models

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ARTICLE INFO

Received Date: 22/08/2025
Accepted Date: 16/11/2025

Cite this paper as:
Parlak,İ.E., Kaykılarlı, C., & Eken, T.Y. (2026). Quantitative Prediction of Ti6Al4V Tribological Behavior Using Advanced Machine Learning Regression with Feature Engineering and Ensemble Models. *Journal of Innovative Science and Engineering.* 10(1), 46-64.

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Keywords:
Ti6Al4V
Machine learning
Artificial intelligence
Tribology
Wear rate
Coefficition of friction

ABSTRACT

The growth of industrial development has increased attention to sustainability and efficiency, resulting in greater research advances toward improved performance of materials. The tribological behavior of materials, specifically friction and wear, is one of the most primary topics of interest in material performance advancement. This work provides an advanced machine learning regression-based model for the quantitative prediction of the Coefficient of Friction (CoF) and wear rate of the Ti6Al4V alloy. The novel approach employs an extensive pipeline of advanced feature engineering to inform an ensemble model based on a dataset compiled from the literature. The optimized Gradient Boosting Regressor achieved F1 results in excess of 95% accuracy on an unseen data set ($R^2 = 0.944$; RMSE = 0.020) for CoF predictions, and a stacking regressor/model markedly improved wear rate predictions ($R^2 = 0.730$) compared to baseline models and the CoF predictions for clarification of real-time engineering applications. The ensemble regression model is designed to provide high-fidelity, quantitative benchmarks for Ti6Al4V, which can be used as critical tools for materials design and optimization. The methodology confirmed the models' important physical relevance through feature-importance analysis: Hardness × Load for the CoF models, and Sliding Distance for wear rate.

1. Introduction

Rapid industrial advancements have substantially increased material and energy consumption, rendering environmental preservation and energy efficiency critical global challenges. Fundamental industrial activities such as transportation, power generation, and manufacturing depend on machinery and mechanical systems comprising numerous interacting surfaces and moving components. Friction and wear are among the primary factors that compromise machine performance, leading to reduced efficiency, increased maintenance expenses, and premature component failure. Consequently, the selection of appropriate materials and the accurate prediction of their friction and wear behaviour are essential for minimising these adverse effects. The reliable, durable, and efficient operation of mechanical systems is intrinsically linked to the effective management of friction and wear at interacting surfaces. Since 1966, the scientific discipline dedicated to investigating and controlling friction, wear, and lubrication in relative motion has been formally recognised as tribology (Menezes et al., 2013; Holmberg & Erdemir, 2017; Wang et al., 2023). Also, Jost described the term "tribology" as the interplay of economic and scientific considerations in the assessment and control of wear, lubrication, and friction on relatively moving contact surfaces (Great Britain Department of Education and Science, 1966). Understanding how materials behave when they slide or roll against each other is essential for improving the design and performance of systems like microelectromechanical systems, machine parts, and human body applications like medical implants (Marian & Tremmel, 2021). Different parameters affect a material's tribological performance—such as the type of wear, the material itself, the counterpart, the load, the material's hardness, the sliding distance, and the speed—which together determine its coefficient of friction (CoF) and wear rate (Hasan et al., 2021).

The new discipline of tribology emerged due to the significant economic impact of wear failures on mid-20th-century British industry. The Jost report highlighted that large-scale adoption of advanced tribological technologies in the UK could save £515 million annually—equivalent to 1.36% of the gross national product (GNP) at the time) within ten years. Following a government investment of £1.25 million in education, research, and industry, the annual savings were later estimated at £200 million (Holmberg & Erdemir, 2017; Great Britain Department of Education and Science, 1966; NBS Special Publication, 1976). Subsequent global studies indicated comparable substantial potential savings, including 2.6% of GNP in Japan (1970), 0.5% in Germany (1976), 0.79–0.84% in the USA (1977, 1981), and 2–7% in China (1986). A study conducted in 2017 indicated that targeted research initiatives in the field of tribology could potentially achieve annual energy savings equivalent to 2.1% of the U.S. GDP. Variations in industrialisation levels, infrastructure, calculation years, and methodologies likely contribute to these differences in the results.

Due to their low density combined with outstanding properties such as chemical resistance, specific strength, and biocompatibility, titanium and its alloys have been the focus of growing scientific interest across a variety of applications (Hayat et al., 2019). The elevated cost, low hardness, restricted wear resistance, and inadequate high-temperature creep resistance of Ti alloys have constrained their widespread application (Kaykılarlı et al., 2025). Thus, the material develops interaction properties such as a highly unstable CoF, a strong attraction for surfaces that causes adhesion and wear, vulnerability to material loss due to fretting, and a tendency for seizure. Ti6Al4V, a multi-phase Ti alloy ($\alpha+\beta$) also known as Ti alloy Ti-6Al-4V, is a widely used engineering, biomedical and research material due to its high strength (higher than that of pure Ti), corrosion resistance, good fatigue resistance, biocompatibility, and low density. It is used in a variety of applications, including the aerospace industry (structural parts, turbine blades), biomedical implants (dental and orthopedic implants), marine engineering, chemical process industries (valves), and sporting equipment (bicycle frames and golf club bats). However, its usability is mainly limited by poor tribological properties and inadequate high-temperature performance. Despite its widespread use, the tribological behavior of Ti6Al4V has not been thoroughly studied. Considering the limited tribological studies on Ti6Al4V, it is essential to conduct further research in this field to bridge the knowledge gap and improve the material's performance in various applications (Philip et al., 2019; Jiang et al., 2023; Pottirayil & Kailas, 2016; Yerramareddy & Bahadur, 1992; Budinski, 1991).

Wear and friction are reactions to the tribo-system rather than inherent features of the material. Assuming that these processes are always linearly related to one another would be incorrect. The two overarching classifications that encompass factors influencing the tribological performance of Ti6Al4V alloys are material variables and tribological test variables. Parameters affecting wear include normal load, sliding velocity, temperature, environment, hardness, elastic modulus, fracture toughness, crystal structure, and thermal diffusivity (Menezes et al., 2013).

The most significant mechanical attribute in classical tribological analysis is frequently regarded as hardness. When two materials interact on a surface, harder alloys show greater cohesion and less adhesion than softer alloys. Due to limited plastic deformability, the deformation component of friction is similarly low for harder alloys. Harder alloys are anticipated to have low overall CoF since they have low adhesion and deformation components of friction. As a result of less adhesive wear, plastic deformation, and material loss, harder materials frequently induce low wear rates during sliding contact. Although there is no clear correlation between sliding distance and CoF, the wear rate rises as the sliding distance does (Quteiro, 2022; Caggiano, 2018; Caggiano, 2018).

The application of machine learning (ML) covers various fields such as finance for credit scoring (Dastile, 2020), healthcare for disease prediction (Uddin, 2019), marketing for customer segmentation (Ozan, 2018), oil and gas industry (Li et al., 2021), food industry (Saha & Manickavasagan, 2021), aviation (Hon et al., 2020), bioengineering and material science (Wang et al., 2023). Recent advancements in ML have significantly progressed material science. These innovations have made it possible to conduct experiments more quickly, find new materials with desired properties more rapidly, establish correlations between various material attributes and their properties, predict material behavior without physical experiments, optimize process parameters and material characteristics, and extract useful information from imaging and spectroscopic data (Ramkumar, 2024). Compared to the conventional experiment-based approach, ML, as a data-driven methodology, supports the simultaneous analysis of numerous variables and facilitates the identification of optimal solutions for enhancing predictive performance (Wang et al., 2023). Despite the limited number of ML uses in tribology, interest has recently increased (Paturi, 2023). By integrating ML algorithms with tribological studies, researchers can more accurately and efficiently predict wear rates and CoF in mechanical systems. This not only improves the performance and reliability of mechanical components, but also contributes to the development of sustainable engineering practices by optimizing maintenance schedules and reducing material waste. The intersection of ML and tribology opens up new frontiers in predictive maintenance, design optimization, and material science. By leveraging the vast data generated in tribological experiments and operations, ML algorithms can uncover complex relationships between operating conditions, material properties, and wear mechanisms. This insight enables the development of more durable materials and lubricants, the design of machines that operate more efficiently, and the creation of maintenance schedules that prevent failures before they occur, thereby extending the lifespan of mechanical systems and contributing to environmental sustainability (Marian & Tremmel, 2021; Shah et al., 2024; Shah et al., 2024).

To accurately predict the tribological performance of Ti6Al4V, it is necessary to consider a range of variables that may affect its CoF and wear rate. These variables may include the hardness of the material as well as the applied load and sliding velocity. Notwithstanding the numerous endeavors to establish principles or laws governing friction and wear, tribology remains an extensively empirical field on account of its intricate nature. However, the abundance of data in tribological research created an opportunity for data-driven analysis. New correlations in data-driven fields are being discovered using ML and artificial intelligence (AI) techniques of "Big Data" analysis, which would be unachievable using the conventional method (Hasan et al. 2021). ML methods might be the answer to this problem because they seem effective at handling the complication of tribological data. As a result, by using such intelligent algorithms in tribology, researchers can better understand tribological occurrences and create a functional connection between process input and output (Paturi, 2023).

Some studies on tribology and ML are available in the literature. (Ramkumar, 2024). prepared Ti-3Al-2.5V-xWC composites via powder metallurgy. To predict the CoF and specific wear rate from experimental results, three ML algorithms—linear regression (LR), decision tree (DT) and random forest (RF)—were used. The findings suggest that the RF model is a useful instrument for forecasting these composites' tribological characteristics. (Jatti et al., 2024) produced a Ti6Al4V composite reinforced with WC and graphite using the stir-casting method and investigated its tribological properties employing ML algorithms such as k-Nearest Neighbor (KNN), Support Vector Machine (SVM), and Extreme Gradient Boosting (XGBoost). The KNN, SVM, and XGBoost algorithms achieved accuracy rates of 71.25%, 65%, and 56.25%, respectively, in predicting the wear rate data. (Hasan et al., 2021) investigated the correlations of friction and wear of Al-based alloys with materials features, heat treatment and processing procedure and tribological test parameters. To predict the wear rates and CoF from tribological experiment data, five different ML algorithms, SVM, Artificial Neural Network (ANN), RF, KNN, and Gradient Boosting Machine (GBM) were used. According to the analysis results, KNN outperformed other ML models for the prediction of CoF. On the other hand, RF exhibited the best accuracy in wear rate prediction. (Wang et al., 2023) investigated tribological performance and wear mechanism of PTFE composites with ML. They used partial squares regression (PLS), Gaussian process regression (GPR), RF and gradient boosting regression (GBR) algorithms for the prediction of the tribological performance and they found that the GBR model showed the best predictive performance for CoF and wear rate. (Jia et al., 2024) produced FeCoCrNiAlN high-entropy coatings and investigated tribological properties. To predict CoF from experimental data, seven different ML algorithms were used: Multiple linear regression (MLR), RF, extra tree (ET), support vector regression radial basis function (SVR.rbf), gradient boosting decision tree (GBDT), and XGBoost. The XGBoost showed the highest accuracy for predicting the CoF.

The application of machine learning in predicting the tribological behavior of titanium alloys is rapidly expanding, though specific studies focusing on the pure Ti6Al4V alloy with advanced regression strategies remain scarce. Mindivan et al. (2025) recently employed a tribo-informatics approach to generate wear maps of the Ti-6Al-4V alloy under dry sliding conditions, primarily focusing on visual representations and descriptive analysis of wear phenomena, which serve as foundational context for data-driven tribology. Separately, the scope of ML in this domain has been expanded to material variants, as shown by (Ramkumar et al., 2025), who investigated the tribological performance of Ti-3Al-2.5V-XWC composites. While these studies affirm the utility of ML in the field, a critical gap remains in achieving highly accurate, continuous quantitative predictions for the standard Ti6Al4V alloy, especially by demonstrating the necessity and effectiveness of advanced modeling techniques. Specifically, most ML-based tribology studies often rely on standard models or simpler classification approaches. Therefore, a study focusing on optimizing prediction performance using state-of-the-art feature engineering and ensemble regression for both CoF and wear rate is necessary to establish reliable quantitative benchmarks for this critical alloy.

This study aims to investigate the effects of material properties and testing parameters on the tribological properties of Ti6Al4V using ML. Firstly, using tribological data reported in the literature for Ti6Al4V, we developed ML algorithms to predict the CoF and wear rate. Finally, we analyzed the performance of different ML algorithms in predicting tribological behavior and presented a comparative analysis of various material and tribological test parameters affecting the tribological performance of Ti6Al4V. As a result of a detailed literature review, it was seen that studies using ML on the tribological properties of Ti6Al4V are extremely limited. Therefore, this study was planned to fill this gap in the literature.

2. Methodology

This study employs a comprehensive machine learning approach to predict the CoF and wear rate of Ti6Al4V alloy through rigorous regression analysis. This approach focuses on continuous value prediction, providing precise quantitative estimates of tribological performance. The methodology encompasses extensive data preprocessing, advanced feature engineering, hyperparameter optimization, and ensemble techniques to maximize the predictive performance and stability of the models.

2.1. Experimental Data and Setup Overview

The foundation of this machine learning study is a meticulously compiled dataset derived from peer-reviewed literature detailing the tribological testing of Ti6Al4V alloy. These data exclusively pertain to experiments conducted using the pin-on-disc setup, employing hardened steel as the counterface material. This specific experimental configuration is visually represented in Figure 1.

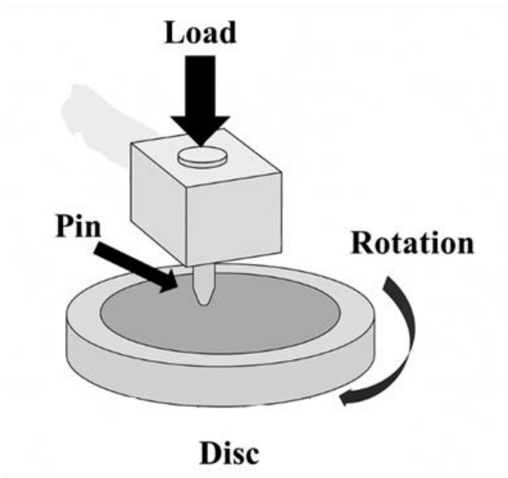

Figure 1: Schematic representation of the pin-on-disc method.

The tribological experiments, as illustrated in Figure 1, typically involve measuring the CoF and wear rate under controlled conditions. The four primary input features extracted from these experiments, which serve as the independent variables for our prediction models, are hardness (HV), load (N), sliding distance (m), and sliding velocity (mm/s).

2.2. Data Collection and Preprocessing

The experimental data utilized in this study were compiled from peer-reviewed literature focusing on tribological testing of Ti6Al4V using pin-on-disc methodology with hardened steel counterparts. The final dataset comprises 62 data points for CoF prediction and 107 data points for wear rate prediction, with four input features: hardness (HV), load (N), sliding distance (m), and sliding velocity (mm/s). Variables in the dataset for CoF and wear rate are shown in Table 1 and Table 2, respectively.

Data preprocessing followed a systematic approach including outlier detection, normalization using min-max scaling (Eq. 1), and train-test splitting with stratification to maintain representative distributions:

$$x' = \frac{x - x_{min}}{x_{max} - x_{min}} \quad (1)$$

where, x represents the raw data value, x' is the normalized value, and x_{min} and x_{max} are the minimum and maximum values respectively.

Table 1: Variables in the dataset for CoF.

Variable	Type of Variable	Unit	Range
Hardness	Input (feature)	HV	280-342
Load	Input (feature)	N	9.81-200
Sliding distance	Input (feature)	m	1000-5520
Sliding velocity	Input (feature)	mm/s	500-4000
COF	Output (target)	-	0.0071-0.493

62 data for CoF

Table 2: Variables in the dataset for waer rate.

Variable	Type of Variable	Unit	Range
Hardness	Input (feature)	HV	218-471
Load	Input (feature)	N	5-200
Sliding distance	Input (feature)	m	600-5520
Sliding velocity	Input (feature)	mm/s	100-4000
Wear rate	Output (target)	mm^3/Nm	0.000015-0.000651

107 data for wear rate

2.3. Machine Learning Pipeline

The comprehensive machine learning approach employed in this study follows a systematic workflow as illustrated in Figure 2. The pipeline incorporates multiple regression algorithms to identify optimal models for each target variable. Fourteen different algorithms were systematically evaluated: Linear Regression (Matter, 2003), Ridge Regression (Hoerl & Kennard, 1970), Lasso Regression (Tibshirani, 1996), Elastic Net (Zou & Hastie, 2005), Decision Trees (Breiman et al., 2001), Random Forest (Breiman, 2001), Extra Trees (Geurts et al., 2006), Gradient Boosting (Friedman, 2001), XGBoost (Chen & Guestrin, 2016), LightGBM (Ke et al., 2017), Support Vector Regression (Drucker et al., 1996), K-Nearest Neighbors (Cover & Hart, 1967), AdaBoost (Freund & Schapire, 1997), and Bagging Regressor (Breiman, 1996).

The cross-validation approach varied based on dataset size, employing 5-fold CV for wear rate prediction and 3-fold CV for CoF prediction to ensure robust model evaluation while maintaining adequate training data (Figure 3). Each fold uses different segments as test data while remaining segments serve as training data. This ensures all data points are used for both training and testing across iterations. Performance metrics included R^2 score, mean squared error (MSE), mean absolute error (MAE), and mean absolute percentage error (MAPE).

2.4. Feature Engineering and Optimization

Advanced feature engineering techniques were implemented to enhance model performance. Polynomial features of degree 2 were generated to capture non-linear interactions between input variables. Additionally, domain-specific engineered features were made based on tribological principles, including the hardness-to-load ratio (material stress factor), sliding work (distance × velocity interaction), load-to-hardness ratio (contact pressure indicator), and velocity-to-distance ratio (sliding intensity).

Hyperparameter optimization was performed using GridSearchCV for smaller datasets and RandomizedSearchCV for larger datasets, with parameter spaces tailored to each algorithm's characteristics.

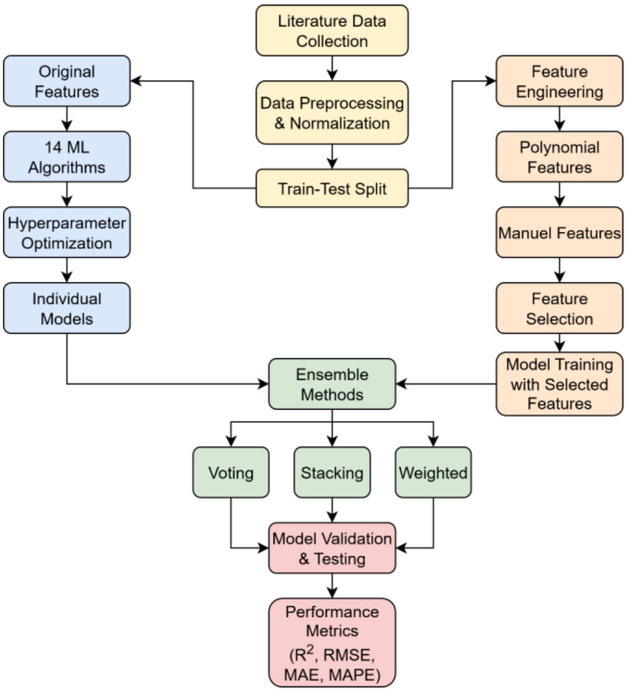

Figure 2: Comprehensive machine learning methodology workflow.

2.5. Ensemble Methods

Three ensemble approaches were evaluated to improve prediction accuracy.

Voting Regressor (Dietterich, 2000) is a simple averaging of predictions from multiple base models; Stacking Regressor (Wolpert, 1992) is a meta-learning approach using linear regression as the final estimator; Weighted Average (Bates & Grager, 1969) is a performance-based weighted combination of predictions.

The ensemble selection was based on cross-validation performance and generalization capability.

2.6. Model Validation and Performance Assessment

Model performance was assessed using multiple metrics to ensure robust evaluation. The coefficient of determination (R^2) served as the primary metric (Eq. 2), supplemented by RMSE for error magnitude assessment (Eq. 3) and MAPE for percentage error evaluation (Eq. 4):

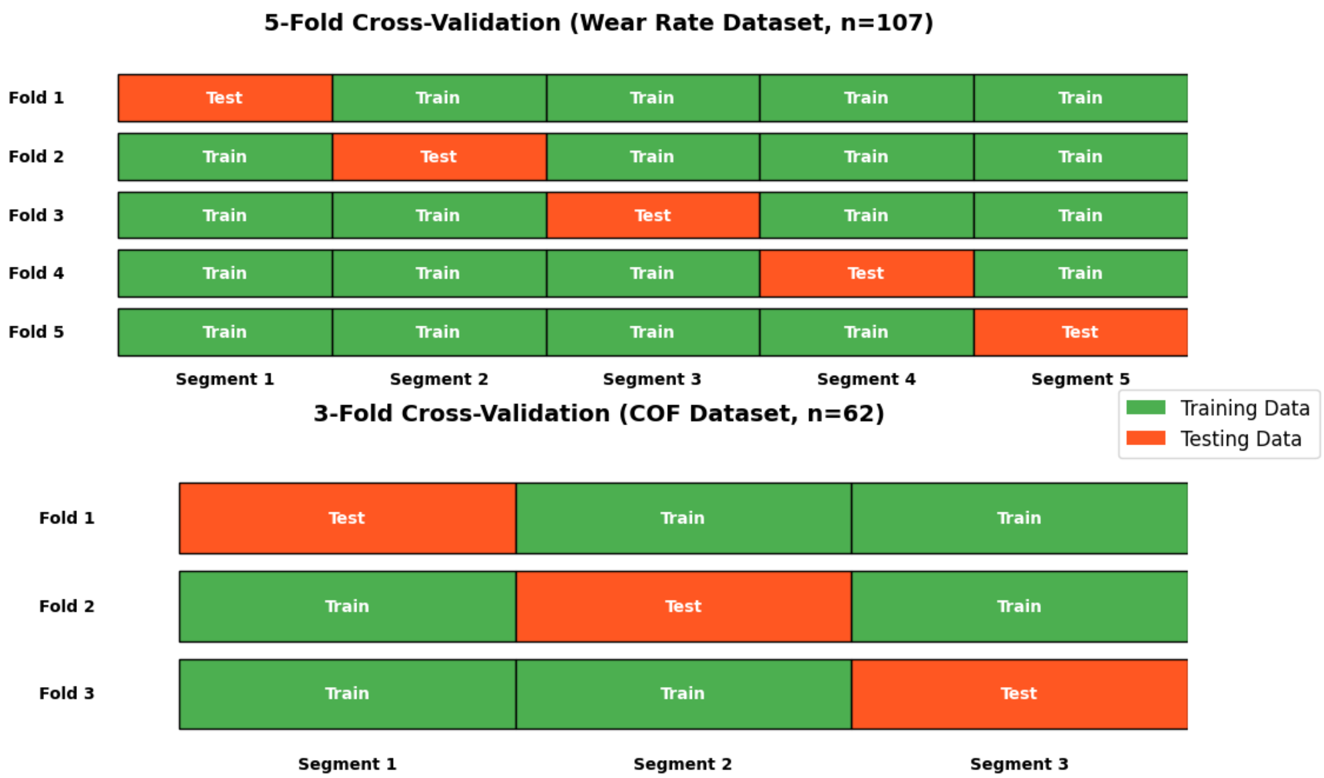

Figure 3: Cross-validation strategies employed for model evaluation and performance assessment.

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}} \quad (2)$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \quad (3)$$

$$MAPE = \frac{100\%}{n}\sum_{i=1}^{n}\left|\frac{y_i - \hat{y}_i}{y_i}\right| \quad (4)$$

where y_i represents actual values, $\hat{y}_i$ represents predicted values, and n is the number of observations.

3. Results

3.1. Dataset Characteristics and Initial Performance

The tribological datasets exhibited distinct characteristics that influenced modeling approaches and outcomes. The CoF dataset comprised 62 experimental observations with target values ranging from 0.007 to 0.493, demonstrating a relatively normal distribution with mean 0.246 and standard deviation 0.099. In contrast, the wear rate dataset contained 107 observations with values ranging from 0.000015 to 0.000651 mm^3/Nm, showing a more skewed distribution characteristic of tribological wear phenomena. The distributional characteristics of both target variables are illustrated in Figures 4 and 5 for CoF and Figures 6 and 7 for wear rate. These include histogram analysis, box plots, logarithmic transformations, and Q-Q plots to assess normality assumptions for subsequent modeling approaches.

Cross-correlation analysis revealed fundamental differences between the two tribological properties. CoF demonstrated a positive correlation with sliding distance (r = 0.546) (Figure 8), while wear rate exhibited a strong negative correlation with the same parameter (r = -0.627) (Figure 9). These opposing relationships reflect the distinct physical mechanisms governing instantaneous friction versus long-term material removal processes.

Initial model evaluation across fourteen algorithms with four scaling approaches yielded markedly different baseline performances. Initial model evaluation across fourteen algorithms established a performance baseline. Figures 10 and 11, which summarize the Test R2 scores for the top-performing model-scaler combinations, illustrate the baseline performance. Table 3 presents the performance comparison of the four most successful algorithms, selected based on their consistent performance across both prediction tasks and scaling methods. For CoF prediction, gradient boosting achieved exceptional baseline performance (R^2 = 0.926) without scaling, indicating strong inherent relationships within the data structure. Conversely, wear rate prediction proved more challenging, with Extra Trees achieving the highest baseline performance (R^2 = 0.597) across all scaling methods, suggesting more complex underlying relationships requiring advanced modeling techniques. Notably, XGBoost demonstrated severe convergence issues for wear rate prediction, achieving negative R^2 scores that indicate performance worse than a simple mean-based predictor.

3.2. Feature Engineering Impact and Optimization

Feature engineering strategies demonstrated varying effectiveness across the two prediction tasks. The quantitative impact of different feature engineering approaches is summarized in Table 4, highlighting the distinct preferences of each prediction task. For CoF prediction, polynomial features of degree 2 provided substantial improvement (R^2 increase from 0.926 to 0.960), while manually engineered tribological features yielded modest gains (R^2 = 0.903). The success of polynomial features suggests that CoF behavior involves significant non-linear interactions between input parameters, particularly the dominant Hardness×Load interaction term. For wear rate prediction, manually engineered features proved more effective than polynomial expansion. The engineered feature set improved performance from R^2 = 0.573 to 0.620, with sliding work (distance×velocity) and hardness-to-load ratio emerging as critical derived parameters. This finding aligns with tribological theory where contact mechanics and energy dissipation govern wear mechanisms.

Hyperparameter optimization revealed algorithm-specific preferences for each dataset. CoF models favored conservative settings due to smaller dataset size, while wear rate models accommodated more complex configurations. XGBoost demonstrated poor convergence for wear rate prediction despite extensive hyperparameter tuning, suggesting fundamental incompatibility with the underlying data structure.

3.3. Ensemble Methods and Final Model Selection

Ensemble approaches yielded contrasting results between the two prediction tasks. For CoF prediction, the optimized single Gradient Boosting model (R^2 =

0.944) outperformed all ensemble methods, including stacking (R^2 = 0.920), voting (R^2 = 0.937), and weighted averaging (R^2 = 0.937). This suggests that CoF relationships are sufficiently well-captured by a single optimized model without requiring ensemble complexity. The comparative performance of ensemble methods for both prediction tasks is illustrated in Figures 12 and 13, demonstrating the superior effectiveness of stacking regression for wear rate prediction while confirming that single optimized models suffice for CoF prediction.

Wear rate prediction benefited significantly from ensemble methods, with stacking regression achieving the highest performance (R^2 = 0.730) compared to the best single model (R^2 = 0.620). The stacking approach effectively combined predictions from the Extra Trees, Gradient Boosting, and Random Forest regressors, leveraging their complementary strengths to capture the complex wear mechanisms.

3.4. Feature Importance and Physical Interpretation

Feature importance analysis revealed distinct driving factors for each tribological property (Figures 14 and 15). CoF prediction was dominated by the Hardness×Load interaction (importance = 0.448), followed by Hardness×Sliding_velocity (0.092) and Load² (0.074), indicating that contact pressure and surface interaction dynamics primarily govern friction behavior.

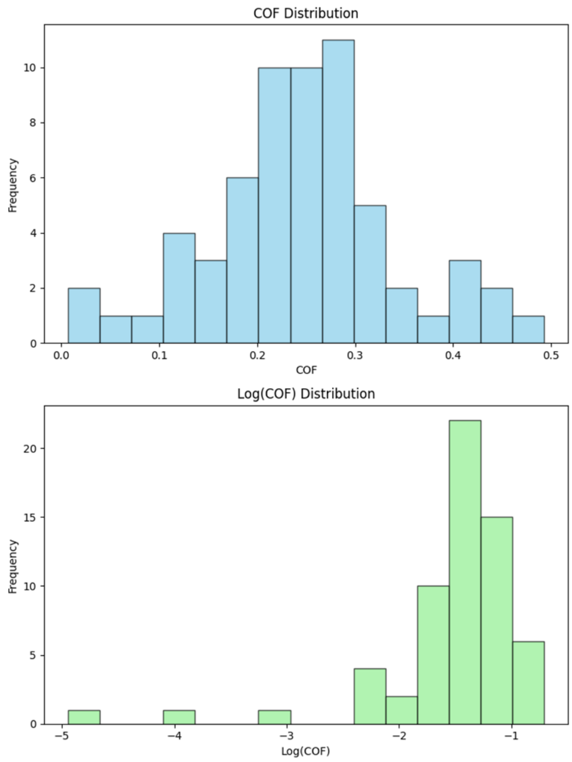

Figure 4: Distribution analysis of the coefficient of friction and primary input features.

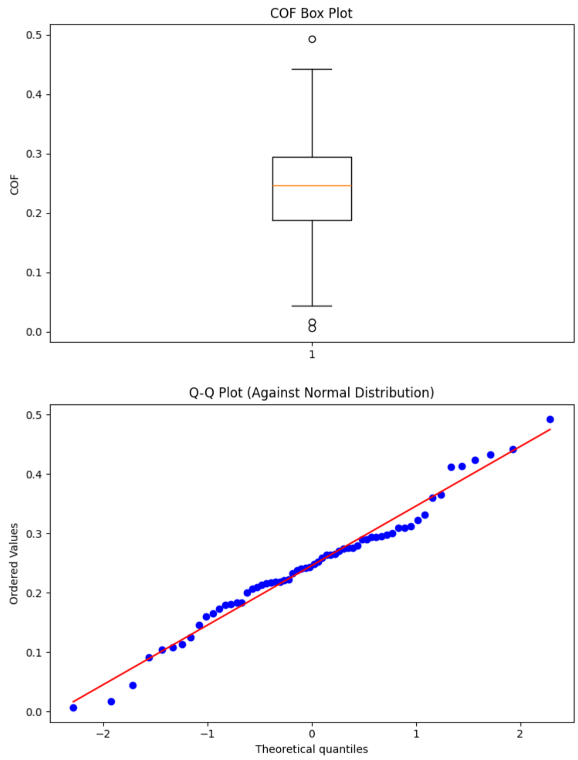

Figure 5: Normality assessment for the CoF.

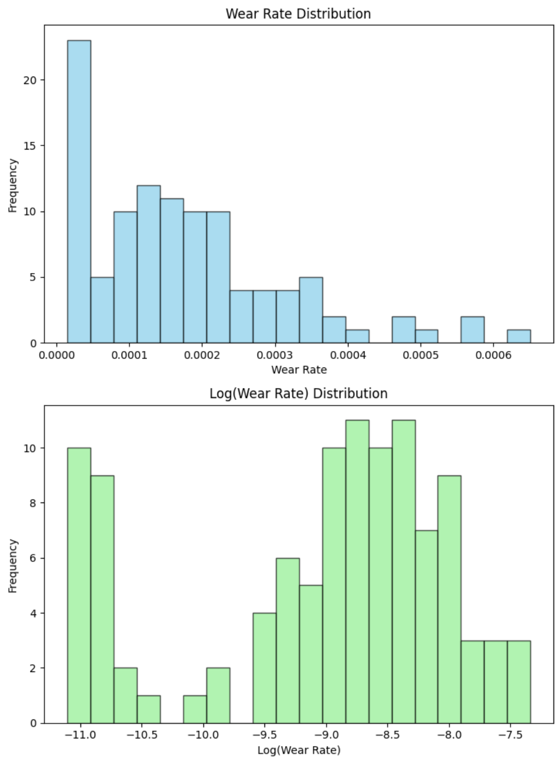

Figure 6: Distribution characteristics for wear rate.

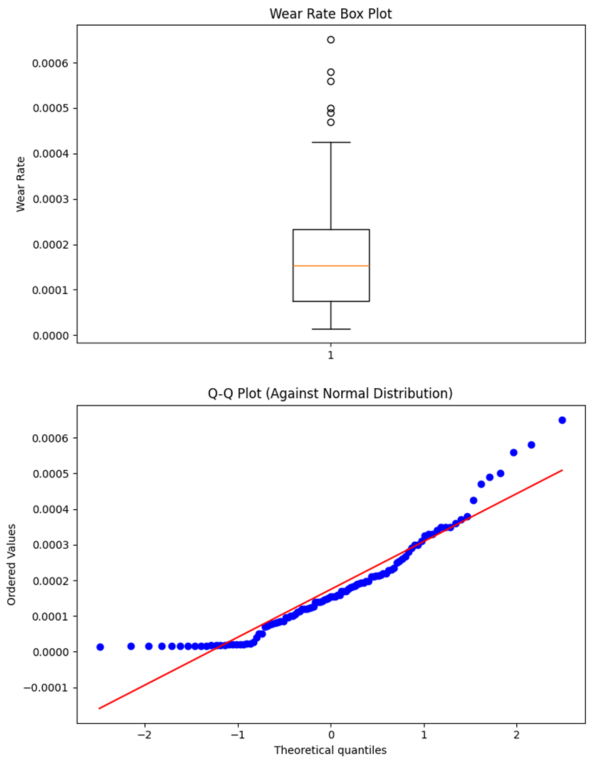

Figure 7: Normality assessment for wear rate.

For wear rate prediction, sliding distance emerged as the most critical factor (importance = 0.317), followed by the hardness-to-load ratio (0.167) and load magnitude (0.149). This hierarchy reflects the cumulative nature of wear processes and the importance of contact stress distribution in material removal mechanisms.

The final optimized models achieved $R^2 = 0.944$ for CoF prediction (RMSE = 0.020, MAPE = 6.5%) and $R^2 = 0.730$ for wear rate prediction (RMSE = 0.000096, MAPE = 57.0%). Model validation through actual versus predicted analysis is presented in Figures 16 and 17, demonstrating excellent prediction accuracy for CoF with minimal residual bias and acceptable performance for wear rate with residuals following approximately normal distribution. The confidence intervals indicate reliable prediction capabilities within the experimental range, with CoF predictions showing tighter bounds reflecting the superior model performance. These performance metrics demonstrate excellent predictive capability for CoF and good performance for wear rate, with the higher error rates in wear rate prediction reflecting the inherently more complex and variable nature of material removal processes.

3.5. Discussion

The contrasting performance outcomes between CoF and wear rate prediction illuminate fundamental differences in the predictability of tribological phenomena. The exceptional accuracy achieved for CoF prediction ($R^2 = 0.944$), compared to the more moderate performance for wear rate prediction ($R^2 = 0.730$), reflects the distinct physical mechanisms governing these properties. CoF represents an instantaneous surface interaction governed by well-defined contact mechanics principles, while wear rate embodies a cumulative material removal process influenced by multiple time-dependent factors including surface fatigue, debris formation, and temperature fluctuations during sliding contact.

Table 3. Baseline performance comparison of top-performing algorithms across CoF and wear rate prediction tasks.

Algorithm	CoF R^2	Wear Rate R^2	CoF CV R^2	Wear Rate CV R^2
Gradient Boosting	**0.926**	0.579	0.754	**0.877**
Extra Trees	0.910	**0.597**	0.742	0.845
XGBoost	0.912	-0.007	0.699	-0.075
Random Forest	0.925	0.508	**0.845**	0.845

Table 4. Impact of Feature Engineering on Model Performance.

Dataset	Original features R^2	Engineered features R^2	Polynomial features R^2	Best approach
CoF	0.926	0.903	0.960	Polynomial
Wear rate	0.573	0.620	0.550	Engineered

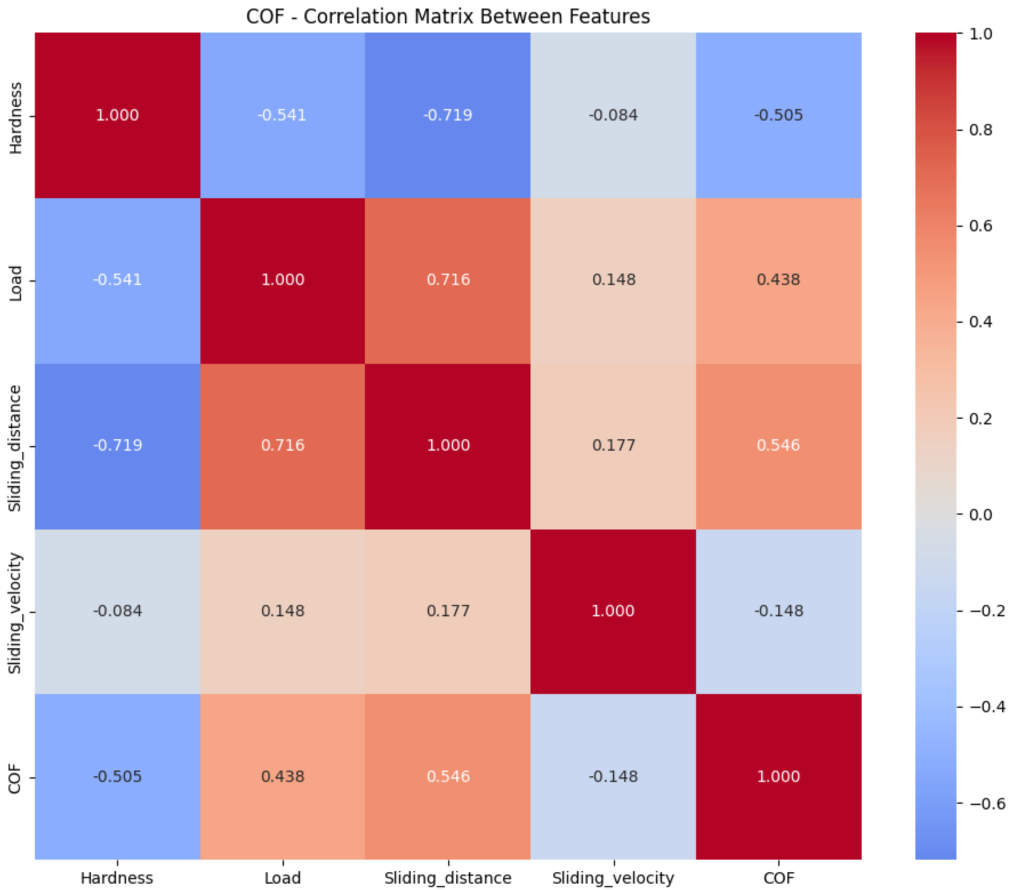

Figure 8: Correlation matrix showing relationships between input parameters and coefficient of friction

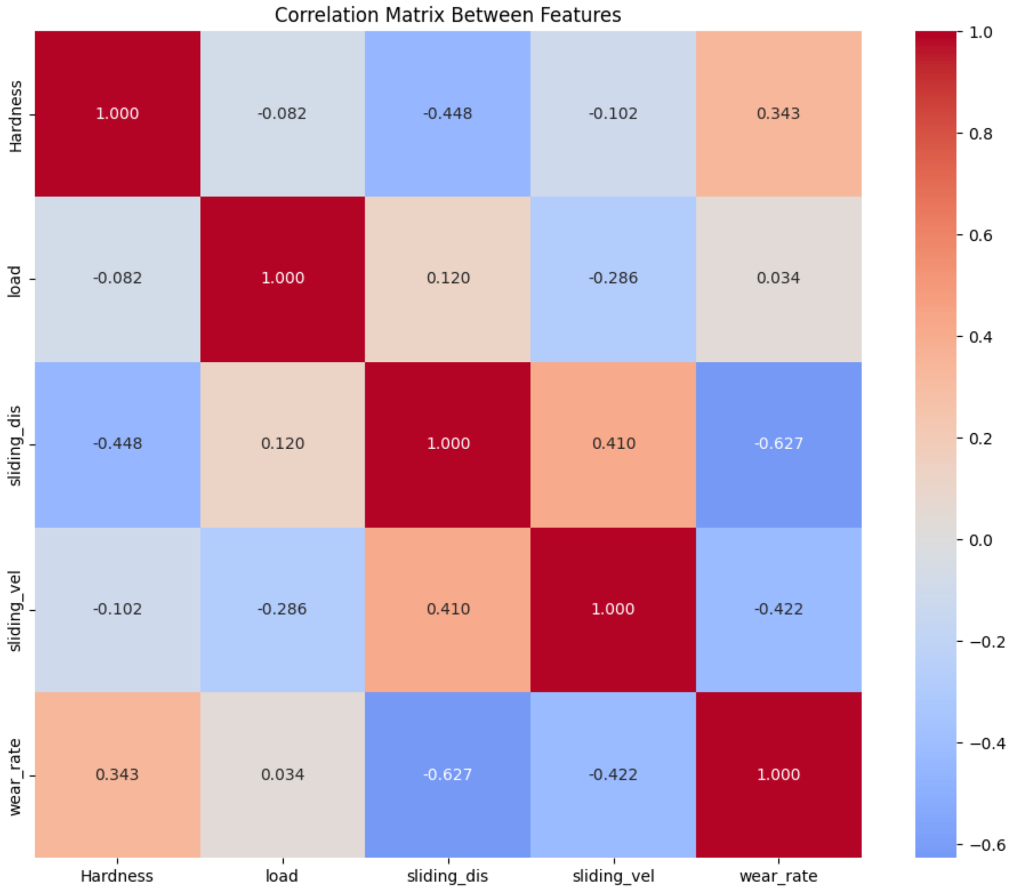

Figure 9: Correlation matrix illustrating parameter interactions in wear rate prediction.

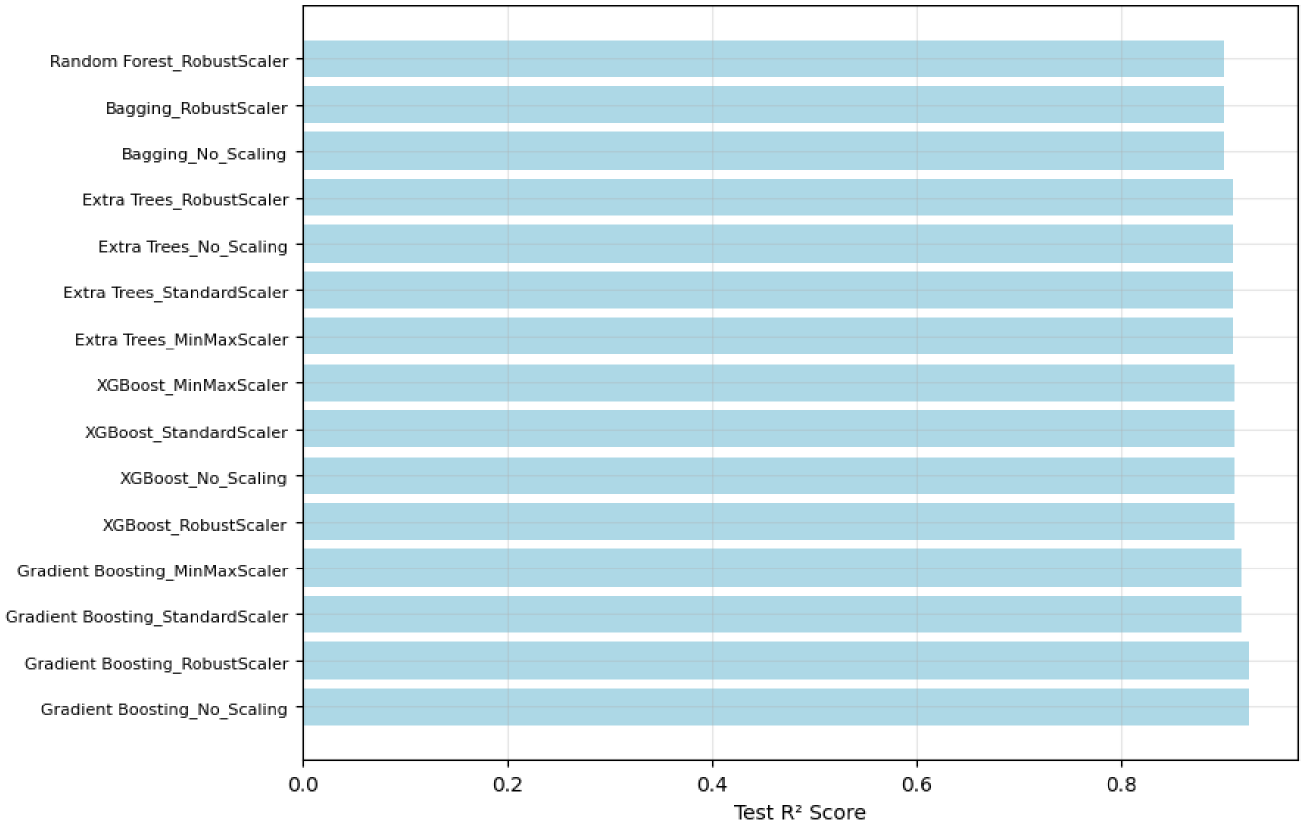

Figure 10: Performance comparison of top 15 machine learning models for coefficient of friction prediction showing test R^2 scores.

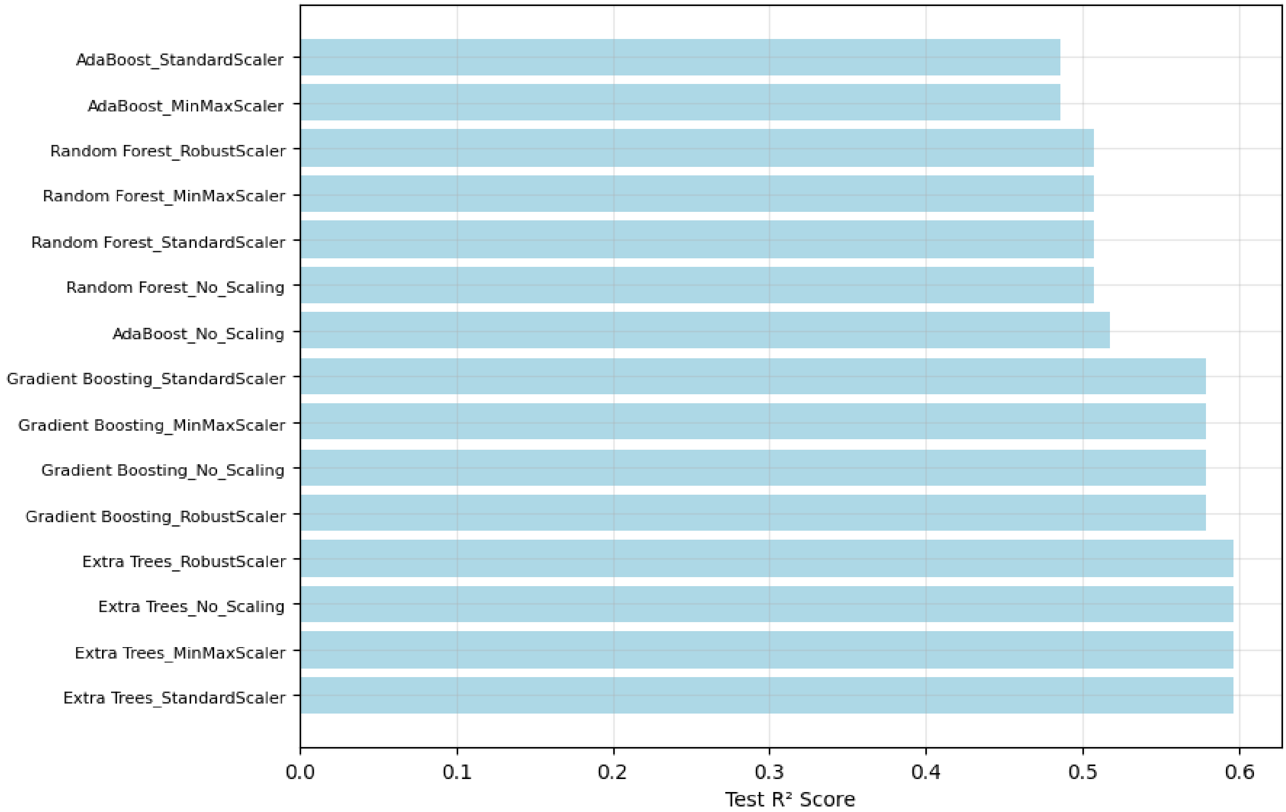

Figure 11: Performance comparison of top 15 machine learning models for wear rate prediction showing test R^2 scores.

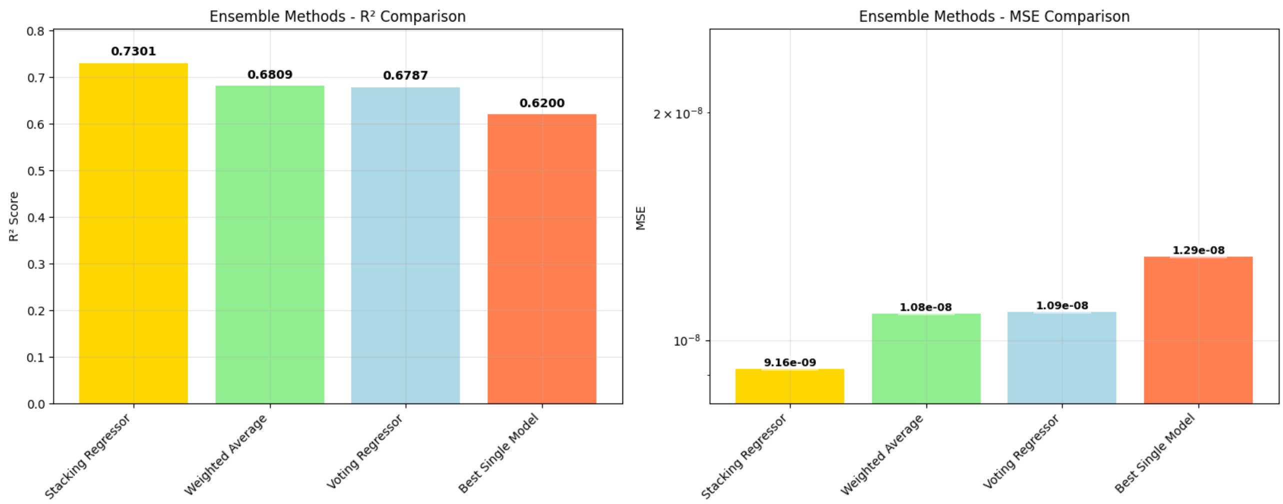

Figure 12: Ensemble methods performance comparison for wear rate prediction showing R^2 scores and MSE values.

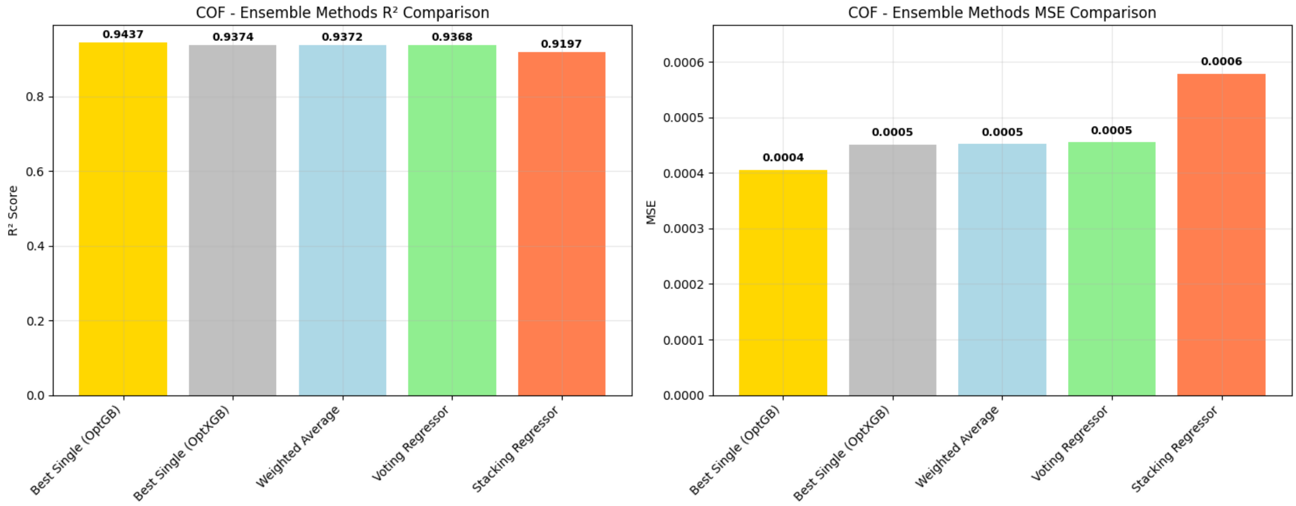

Figure 13: Ensemble methods performance comparison for CoF prediction showing R^2 scores and MSE values.

The final optimized models achieved $R^2 = 0.944$ for CoF prediction (RMSE = 0.020, MAPE = 6.5%) and $R^2 = 0.730$ for wear rate prediction (RMSE = 0.000096, MAPE = 57.0%). Model validation through actual versus predicted analysis is presented in Figures 16 and 17, demonstrating excellent prediction accuracy for CoF with minimal residual bias and acceptable performance for wear rate with residuals following approximately normal distribution. The confidence intervals indicate reliable prediction capabilities within the experimental range, with CoF predictions showing tighter bounds reflecting the superior model performance. These performance metrics demonstrate excellent predictive capability for CoF and good performance for wear rate, with the higher error rates in wear rate prediction reflecting the inherently more complex and variable nature of material removal processes.

3.6. Discussion

The contrasting performance outcomes between CoF and wear rate prediction illuminate fundamental differences in the predictability of tribological phenomena. The exceptional accuracy achieved for CoF prediction ($R^2 = 0.944$) compared to the moderate success for wear rate prediction ($R^2 = 0.730$) reflects the distinct physical mechanisms governing these properties. CoF represents an instantaneous surface interaction governed by well-defined contact mechanics principles, while wear rate embodies a cumulative material removal process influenced by multiple time-dependent factors including surface fatigue, debris formation, and temperature fluctuations during sliding contact.

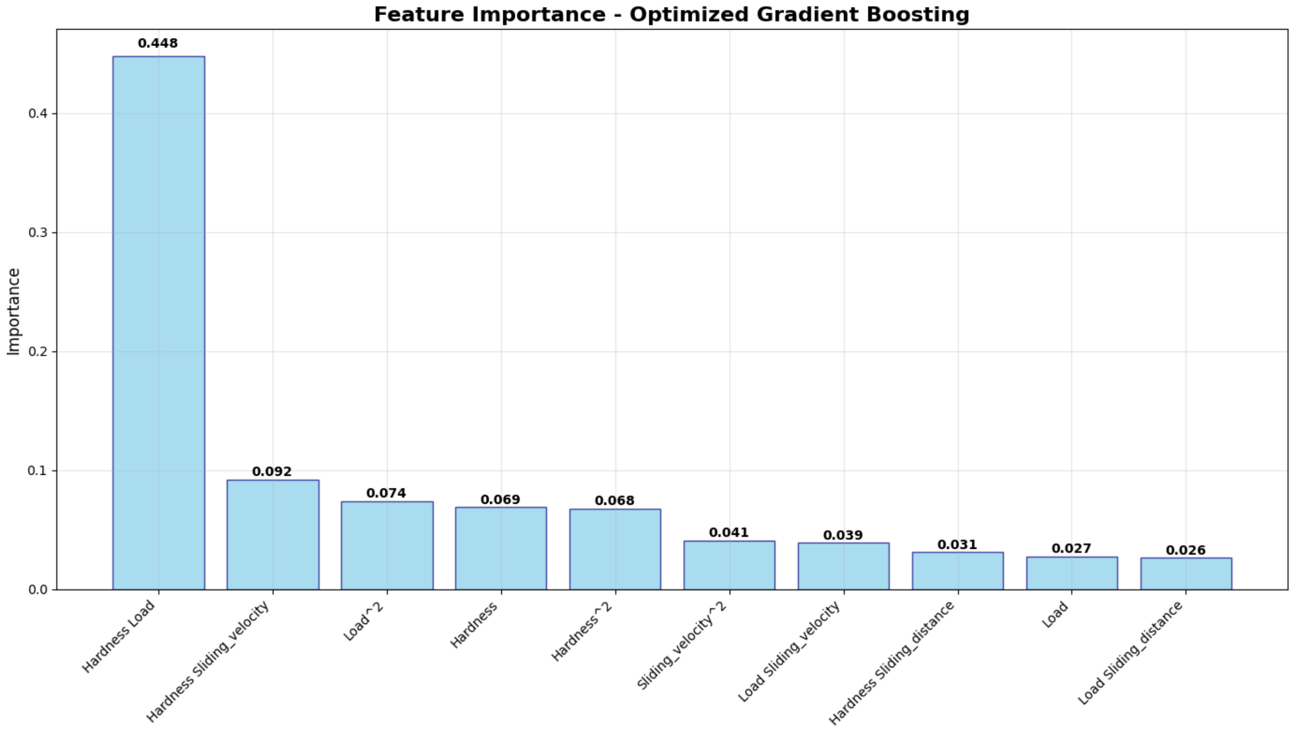

Figure 14: CoF feature importance.

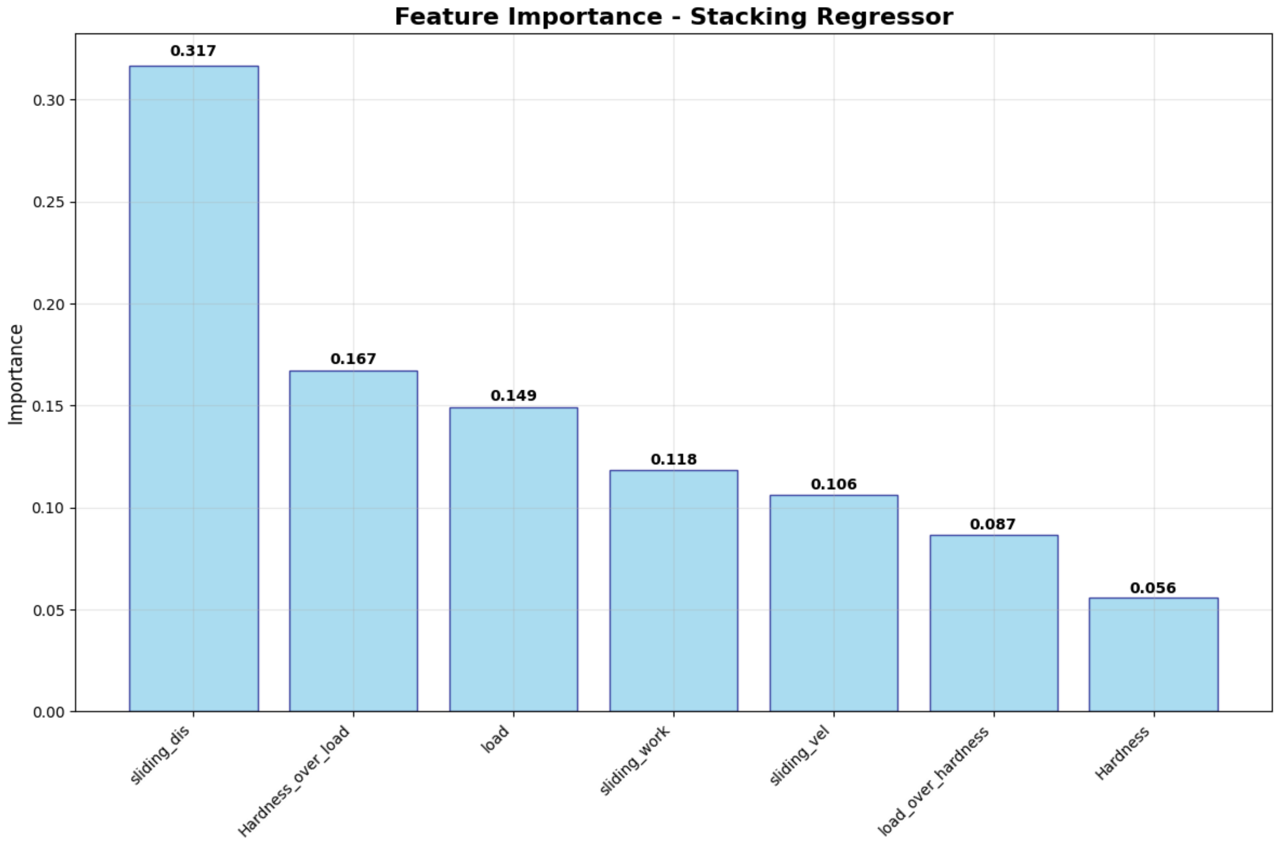

Figure 15: Wear rate feature importance.

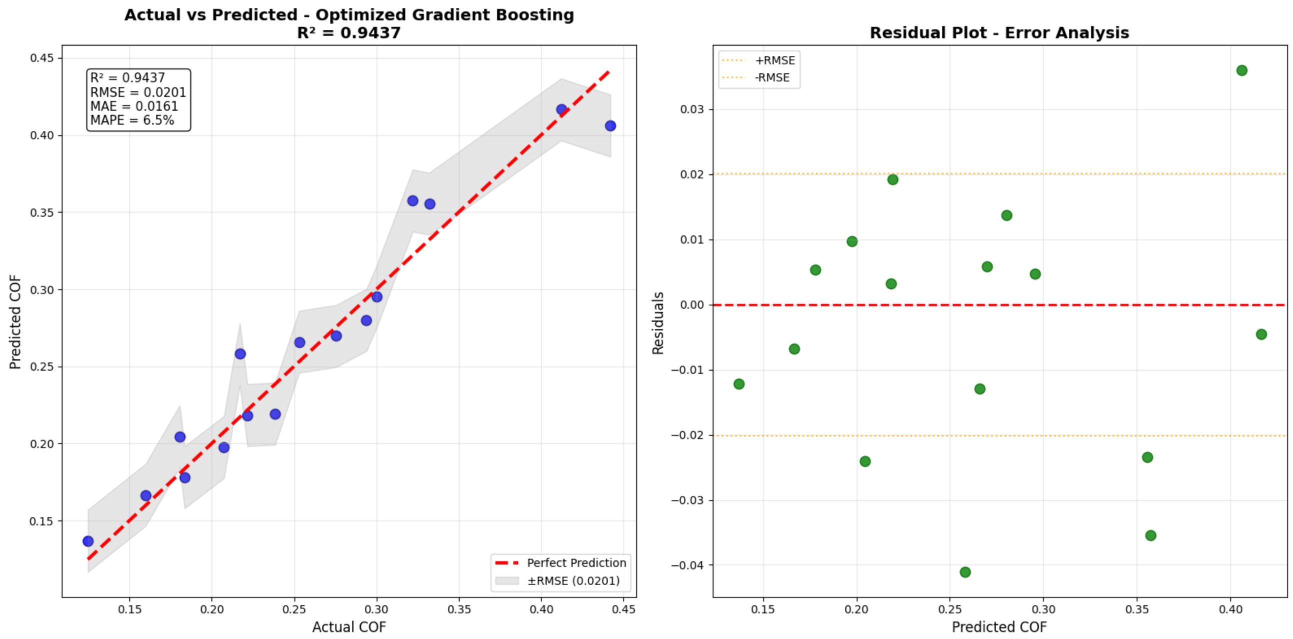

Figure 16: Model validation for CoF prediction: actual vs predicted values with confidence intervals and residual analysis showing error distribution.

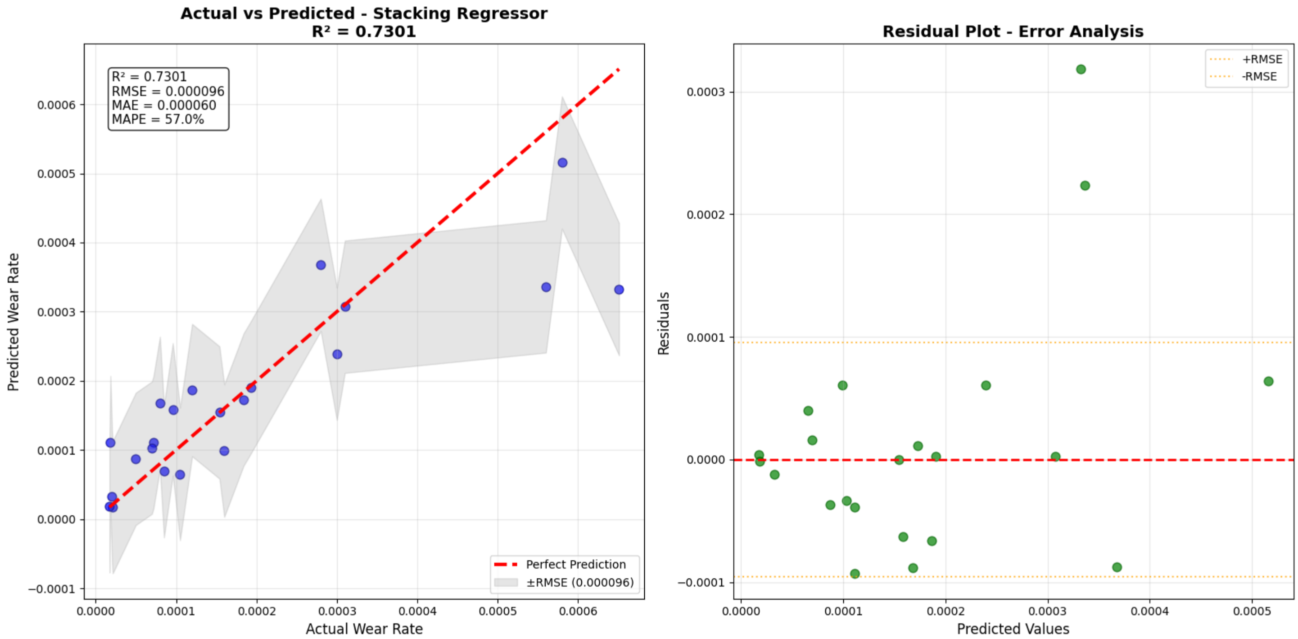

Figure 17: Model validation for wear rate prediction: actual vs predicted values with confidence intervals and residual analysis showing error distribution.

The dominance of polynomial features in CoF modeling, particularly the Hardness×Load interaction term, aligns with established tribological theory where contact pressure serves as the primary determinant of friction behavior. This finding supports Hertzian contact mechanics principles and validates the physical relevance of the machine learning approach. Conversely, the effectiveness of manually engineered features for wear rate prediction suggests that domain expertise remains crucial for capturing the complex interdependencies in material removal processes.

The failure of XGBoost for wear rate prediction, despite its widespread success in other domains, highlights the importance of algorithm selection based on data characteristics rather than general reputation. The negative R^2 values indicate fundamental incompatibility between XGBoost's optimization approach and the wear rate data structure, possibly due to the algorithm's sensitivity to outliers or specific distributional assumptions that are violated in tribological data.

Ensemble methods demonstrated task-specific effectiveness, with stacking regression proving essential for wear rate prediction while offering minimal benefit for CoF prediction. This divergence suggests that CoF relationships are sufficiently well-captured by single optimized models, whereas wear rate prediction benefits from combining multiple algorithmic perspectives to handle the inherent complexity and variability in material removal mechanisms.

The significant difference in MAPE values between CoF (6.5%) and wear rate (57.0%) predictions warrants consideration for practical applications. While both models achieve acceptable R^2 scores, the higher percentage errors in wear rate prediction reflect the challenging nature of quantitative wear prediction and suggest that interval predictions or uncertainty quantification may be more appropriate for industrial applications.

Dataset size limitations, particularly for CoF prediction with only 62 observations, constrained the application of advanced deep learning approaches and limited cross-validation strategies. Future work should prioritize data collection to enable more robust model development and validation. The successful performance achieved despite these limitations demonstrates the effectiveness of the employed feature engineering and ensemble strategies for small dataset scenarios.

The physical interpretation of feature importance rankings provides valuable insights for tribological system design. The critical role of sliding distance in wear rate prediction confirms the cumulative nature of material removal, while the prominence of hardness-load interactions in both predictions emphasizes the fundamental importance of contact mechanics in tribological performance optimization.

A significant methodological distinction of this study is the construction of the dataset from diverse peer-reviewed literature sources, rather than a single, controlled experimental campaign. This approach provides two distinct advantages: enhanced model generalizability by spanning a wider range of experimental conditions (Load, Speed, Hardness) and increased robustness by minimizing the bias inherent in data originating from one lab or setup. However, this method also introduces inherent challenges, primarily concerning data heterogeneity and potential measurement inconsistencies between sources. The relatively small dataset size (CoF: 62, Wear Rate: 107) is a direct consequence of this literature compilation approach. The successful performance achieved, particularly the high R^2 scores derived from the use of advanced feature engineering and ensemble strategies, validates that this methodology is effective in extracting meaningful, generalizable predictive power from small, disparate tribological data pools.

4. Conclusion

This study successfully implemented an advanced machine learning approach that applies rigorous regression analysis for the quantitative prediction of the coefficient of friction and wear rate of the Ti6Al4V alloy. By transitioning from a binary classification approach to continuous value prediction, this work significantly enhanced the predictive capability, providing high-fidelity numerical estimates crucial for material science applications. The adopted methodology successfully navigated the challenges posed by the small, literature-derived dataset, primarily through the systematic application of sophisticated feature engineering, hyperparameter optimization, and ensemble methods.

The final optimized models demonstrated exceptional performance across both tribological properties. The Optimized Gradient Boosting Regressor achieved an outstanding R^2 score of 0.944 (RMSE = 0.020) for CoF prediction, validating the strength of a single optimized model in capturing stable friction dynamics. Conversely, the prediction of the inherently more complex wear rate was significantly enhanced only after the deployment of an Ensemble Stacking Regressor, which elevated the R^2 score to 0.730. This methodological divergence highlights that while CoF relationships can be captured by single, optimized models, modeling the high variability of cumulative wear processes necessitates combining complementary algorithmic perspectives. Furthermore, the effectiveness of Feature Engineering proved critical: CoF prediction was dominated by polynomial features (e.g., Hardness × Load), reinforcing the role of non-linear contact mechanics, whereas domain-specific engineered features such as Sliding Work were essential for achieving robust prediction for wear rate.

Feature importance analysis provided valuable physical insights, confirming the physical relevance of the resulting models. The wear rate model established that the property is primarily governed by the cumulative effect of sliding distance, while CoF is determined by contact pressure (Hardness × Load). In conclusion, this research successfully demonstrates the potential of utilizing advanced regression strategies and tribologically informed feature engineering to derive accurate quantitative models for Ti6Al4V tribological behavior, offering crucial tools for material design optimization. Moving forward, future work should prioritize expanding the size and scope of the experimental data to further improve the generalization capacity of the models. Crucially, the next phase of this research will involve the experimental validation of the developed models through different experimental designs, ensuring the robustness and reliability of the machine learning predictions. Additionally, the successful prediction results achieved in this study open the path for utilizing the established machine learning models in inverse design, where the models can be run in reverse to identify the optimal current input parameters (e.g., Load, Hardness) required to produce materials with desired CoF and wear rate values.

Article Information

Financial Disclosure: The author (s) has no received any financial support for the research, authorship or publication of this study.

Authors' Contrtibution: The authors contributed equally to the study.

Conflict of Interest/Common Interest: No conflict of interest or common interest has been declared by the authors.

Ethics Committee Approval: Ethics committee approval was not applicable to this study.

Data availability statement: Data are available from the authors upon reasonable request.

Artificial Intelligence Statement: The author(s) bear full responsibility for the content and accuracy of their work, including any use of artificial intelligence (AI) technologies, and confirm that they have read the AI Policy, which is accessible on the journal's website.

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