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Fatigue Strength Prediction using Machine Learning in Steels

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ABSTRACT

Fatigue strength is an intrinsic mechanical characteristic that predicts the endurance of materials under repeated cyclic stresses over a period. Predicting fatigue behaviour accurately is important to avoid early failure in essential applications like aerospace, automotive, and structural engineering. This project focuses on the significance of estimating rotating bending fatigue strength on the basis of material composition, heat treatment characteristics, and microstructural inclusion properties. In order to capture the multifaceted, non-linear dependencies among these variables and fatigue performance, various regression models have been employed, i.e., Gradient Boosting, XGBoost, Random Forest (MS), and Linear Regression. All these models reflect different insights of learning patterns from the dataset and help in mapping the prediction landscape. Missing or undefined user input is handled through K-Nearest Neighbours (KNN) imputation so fatigue strength can be estimated even from incomplete data. Users input known parameters like carbon content, alloying elements, heat treatment information, and inclusion information and the model estimate the fatigue strength accordingly. This model facilitates flexible, data-driven decision-making in material design and evaluation procedures.

Keywords: Fatigue Strength Prediction, Material Composition, Heat Treatment Parameters, KNN Imputation.

1. Introduction

Fatigue failure is an important problem that affects the durability of materials used in structures and aerospace applications. It happens when materials are subjected to repeated stresses that are lower than their maximum strength, causing cracks to form and grow over time. Predicting fatigue strength accurately is very important in industries like aerospace, automotive, biomedical, and structural engineering because failures can lead to serious consequences. Traditional fatigue testing methods take a long time and require complete information about the material and processing conditions, which is often not available during early stages of development. Machine learning offers a useful alternative by predicting fatigue behaviour using data on material composition, heat treatment, and microstructure.

This project develops an intelligent system that uses several machine learning models, such as Gradient Boosting, XGBoost, Random Forest, and Linear Regression, trained on detailed datasets of material properties. To handle missing information, the system applies K-Nearest Neighbours (KNN) imputation, allowing it to provide reliable fatigue strength predictions even when some input data is not known. The models are evaluated using standard performance metrics to identify their strengths, rather than relying on a single best model. This approach provides engineers with a practical tool that combines predictive analytics and material science, improving decision-making by delivering accurate fatigue strength estimates from partial or full data. By integrating Explainable AI methods, the system also enhances transparency, allowing users to understand the key factors influencing each prediction. This makes the tool not only predictive but also informative, enabling more confident and informed engineering decisions.

Nomenclature

NT : Normalizing Temperature THT : Through Hardening Temperature THt : Through Hardening Time THQCr : Cooling Rate for Through Hardening CT : Carburization Temperature Ct : Carburization Time DT : Diffusion Temperature Dt : Diffusion Time QmT : Quenching Media Temperature (for Carburization) TT : Tempering Temperature Tt : Tempering Time TCr : Cooling Rate for Tempering RedRatio : Reduction Ratio (from ingot to bar) dA : Area proportion of inclusions deformed by plastic work dB : Area proportion of inclusions occurring in discontinuous array dC : Area proportion of isolated inclusions Fatigue : Rotating Bending Fatigue Strength (10⁷ Cycles) MSE : Mean Squared Error (evaluation metric) R² : Coefficient of Determination (evaluation metric) R² : Coefficient of Determination (evaluation metric) GB : Gradient Boosting (regression model) RF : Random Forest (regression model) XGBoost : Extreme Gradient Boosting (regression model) SVR : Support Vector Regression (used in referenced studies) LSTM : Long Short-Term Memory (deep learning model for sequence prediction)

1.1 Problem Statement

Fatigue failure is a leading cause of damage in critical engineering components subjected to repeated stresses over time. Traditional fatigue strength prediction relies on lengthy, costly physical testing and complete material data, which limits its practicality and flexibility. These methods also struggle with missing data and complex relationships between material composition, processing, and microstructure. With increasing material complexity, there is a need for prediction systems that can accurately estimate fatigue strength even with partial or uncertain input. This project develops an AI-based system using advanced machine learning and K-Nearest Neighbours imputation to predict rotating bending fatigue strength from partial or full user inputs. The system improves decision-making by reducing dependence on extensive experiments, speeding up prototyping, and enabling safer, more cost-effective engineering designs. It also provides a user-friendly interface for engineers to easily input known values and receive reliable predictions. Overall, the system brings a smart, adaptable approach to modern fatigue strength evaluation.

1.2 Proposed System

The proposed fatigue strength prediction system is designed to provide a reliable, flexible, and intelligent solution for estimating how materials perform under repeated cyclic stresses. It uses advanced machine learning, specifically Gradient Boosting, to model the complex relationships between material composition, heat treatment conditions, and microstructural features. Unlike traditional methods that require complete data, this system is trained on both full and partial datasets, allowing it to maintain strong predictive performance even when some inputs are missing. This makes it particularly useful during the early stages of material design or failure analysis when not all information is readily available.

The system allows users to input known material properties, such as carbon content, alloying elements, heat treatment parameters, and inclusion characteristics. If some of these inputs are unavailable, it automatically uses K-Nearest Neighbours (KNN) imputation to estimate the missing values and still deliver accurate fatigue strength predictions. This ensures that engineers can work with whatever information is at hand without compromising on reliability. In addition, the model integrates explainable AI techniques, making the decision-making process transparent and easier to understand. Overall, this system enhances the way engineers select and evaluate materials, supports faster prototyping, and helps reduce the risk of fatigue-related failures in critical applications like aerospace, automotive, and structural engineering.

1.3 Existing System and its disadvantages

Conventional methods for predicting fatigue strength mainly rely on empirical models, standardized fatigue tests, and experiment-based reference tables. These approaches require complete and precise input data such as detailed chemical composition, heat treatment conditions, and microstructural information to deliver accurate predictions. However, such detailed information is often unavailable during early design or material selection phases. Additionally, these traditional systems are not flexible enough to handle missing or partially known data, which limits their usefulness in real-world situations where some material properties may be uncertain or incomplete. Most existing fatigue prediction tools are either too generalized or based on limited datasets, often assuming simple linear relationships between material inputs and fatigue life. They typically fail to capture the complex, non-linear interactions between alloy elements, heat treatments, and inclusion characteristics, reducing their accuracy and reliability. These limitations make current fatigue strength prediction systems outdated and inadequate for today's engineering challenges. They rely heavily on full datasets and can produce inaccurate or unusable results if any material parameter is missing or only partially known, which is common during initial design stages. Moreover, these traditional models lack the ability to explain how predictions are made, reducing engineers' trust and confidence in the results. They also do not support interactive features like "what-if" analyses or adaptive learning, making them inflexible and unable to evolve with new data or user needs. Overall, these systems are rigid and limited, falling short of providing transparent, user-friendly, and accurate fatigue strength predictions needed for advanced material design and modern engineering applications.

2. Literature Survey

Jiang Chang et al. (2025) proposed a hybrid approach that integrates physics-based fatigue life models with machine learning (ML) techniques to quantify uncertainty in fatigue predictions for metal alloys. Their study emphasized the importance of validating uncertainty intervals for improved prediction consistency. Michael Foster et al. (2025) introduced the use of LSTM neural networks to model fatigue crack propagation under variable loading conditions in aerospace alloys. This model captured temporal stress patterns effectively but required large, structured datasets. Yongjie Liu et al. (2024) applied XGBoost regression to predict yield strength and ultimate tensile strength in 7050 aluminum forgings, identifying second-stage aging time as a crucial factor. Hiroshi Tanaka et al. (2024) focused on low-carbon steels and demonstrated high predictive accuracy when the ML model was trained with clean, high-resolution data, stressing the impact of data quality. Laura Stein et al. (2024) employed Gradient Boosting and XGBoost to investigate how inclusion content and reduction ratios influence fatigue strength, revealing nonlinear dependencies but also reporting high computational demands during feature selection. Min Yi et al. (2023) used neural networks and random forests to estimate fatigue life in additively manufactured (AM) materials, highlighting the dependency on dataset quality. Sandra Lee et al. (2023) applied random forest and support vector regression to analyze how carbide precipitation affects fatigue resistance, noting challenges in interpretability. Chen Liu et al. (2023) developed an interpretable fatigue prediction model for steels by combining SHAP analysis with Random Forest, offering both high accuracy and insights into feature importance. Guo et al. (2023) proposed a Bayesian-optimized Random Forest model for ferrous alloys that enhanced both accuracy and generalization while integrating prediction uncertainty. A. Q. Khan et al. (2023) correlated microstructural morphology with fatigue behavior in low-alloy steels using image-derived features. F. B. Machado et al. (2021) studied surface integrity effects on hardened steels and emphasized the significance of machining-induced microstructural deformation. A. Patel and S. Shah (2021) analyzed how alloying elements like chromium and molybdenum impact tool steel fatigue, confirming strong predictive correlations. J. Chen and Y. Liu (2021) applied a physics-guided ML approach to estimate fatigue in AM Ti-6Al-4V alloys, integrating empirical laws with learning models. K. Singh et al. (2020) explored the effect of inclusion morphology in clean steels and demonstrated how elongated oxides diminish fatigue life. Finally, P. Kumar and N. Yadav (2020) investigated carburization and quenching in medium-carbon steels, with ML models effectively capturing their influence on fatigue performance.

3. Design and Methodology

The development of the fatigue strength prediction model begins with an extensive data gathering phase, where key material parameters are collected. These include chemical composition elements such as Silicon, Carbon, and Manganese, along with heat treatment conditions and microstructural inclusion characteristics. Operational features like Normalizing and Tempering Temperatures, Carburization Times, and Hardening Durations are included to ensure a comprehensive dataset that captures all significant factors influencing fatigue behaviour under cyclic loading.

The next crucial step is data preprocessing, which focuses on improving the dataset's quality and consistency. Irrelevant or redundant features are removed to streamline the data. Missing values, which are common in real-world datasets, are handled through K-Nearest Neighbours (KNN) imputation, preserving the integrity of the dataset. Categorical variables are numerically encoded, outliers are corrected, and all features are scaled and normalized to ensure uniform contribution during training. Feature selection and engineering follow, where the most impactful attributes are retained and new derived features are generated to expose hidden relationships. This improves both the model's efficiency and its predictive power.

Model training is carried out using a Gradient Boosting Regressor due to its robustness in modelling complex, nonlinear dependencies between input parameters and fatigue strength. Hyperparameter tuning—such as adjusting the number of estimators and maximum depth—is employed to further enhance the model's performance. The trained model is then evaluated using performance metrics like Mean Squared Error (MSE) and R-squared (R²), ensuring its effectiveness on unseen data. In the prediction phase, the model accepts both complete and incomplete user input, using KNN to impute missing values automatically. This capability makes the system highly adaptable to real-world scenarios. Additionally, Explainable AI techniques are integrated to offer transparency in predictions, helping users understand the influence of each feature. To ensure long-term reliability, the model incorporates continuous monitoring and feedback loops, allowing it to evolve with advancements in material science and manufacturing, thereby maintaining high accuracy over time.



Fig. 1 - Flow Diagram Representation of Fatigue Strength Prediction Model

4. Architecture and Algorithm

The design of the fatigue strength prediction system follows a methodical and logically structured sequence, as illustrated in Fig.2. This architecture ensures that the system produces accurate and consistent results regardless of whether the user provides complete or partial input data. Initially, users are prompted to enter essential material properties such as chemical composition (e.g., carbon, silicon, manganese), alloying elements, heat treatment parameters (like normalizing temperature and tempering time), and microstructural features (such as inclusion area fractions). These parameters form the foundation for fatigue strength prediction, as the system utilizes them to estimate the material's behaviour under rotating bending conditions.

Upon data submission, the system addresses any missing or undefined values through K-Nearest Neighbours (KNN) imputation, ensuring that incomplete entries do not compromise prediction accuracy. This step preserves data integrity and maintains model robustness. The completed dataset is then subjected to scaling and standardization processes to ensure all features contribute equally to the model's performance, avoiding biases from attributes with larger numerical ranges. The pre-processed data is subsequently passed to a trained Gradient Boosting model, which has learned complex, non-linear relationships from historical datasets. The model outputs a predicted value for fatigue strength, which is then presented to the user as a reliable estimation of the material's durability under cyclic loading.

The system's user-centric design ensures flexibility and accessibility for various user scenarios, including cases where only partial information is available. Its built-in adaptability and intelligent handling of incomplete data make it highly practical for early-stage design or rapid material screening. Furthermore, the application of machine learning allows the model to continuously improve and generalize across diverse material combinations. This empowers engineers, designers, and researchers to make well-informed decisions about material selection and structural design while significantly reducing the risk of fatigue-related failures in critical components.



Fig. 2 - Flow diagram for Architecture of the Model.

4.1 Gradient Boosting

Gradient Boosting (GB) is a highly effective ensemble machine learning technique widely used for both regression and classification tasks. It operates by combining the predictions of multiple weak learners—typically shallow decision trees—into a strong learner through a process of iterative improvement. Each new tree is trained to correct the prediction errors made by the ensemble of trees built so far. This is achieved by optimizing a loss function through gradient descent. A key strength of Gradient Boosting lies in its focus on learning from the hardest-to-predict instances. During each iteration, the model calculates the gradients (residual errors) of the loss function and uses these gradients to fit the next tree. This makes GB particularly adept at capturing intricate, nonlinear patterns in data, which is essential in applications such as fatigue strength prediction, where the relationships between material properties, processing parameters, and performance are highly complex and not easily modelled with linear techniques.

Moreover, Gradient Boosting provides a variety of hyperparameters to fine-tune the learning process and prevent overfitting. These include:

- Number of estimators (trees): Controls how many trees are added sequentially.
- Tree depth: Determines the complexity of each tree; deeper trees can model more complex interactions.
- Learning rate: Scales the contribution of each tree, helping balance the speed of learning with stability.
- Subsample ratio: Allows random subsampling of the data for each tree to introduce variance and reduce overfitting.
- Regularization parameters: Such as min_samples_split or min_samples_leaf control tree growth and generalization.

5. Implementation and Results

The proposed fatigue strength prediction system is designed to estimate rotating bending fatigue strength based on user-provided or partially known material inputs. The model incorporates Gradient Boosting Regressor, a powerful ensemble learning method that builds decision trees sequentially to minimize residual errors and capture complex non-linear patterns among features. The model was trained on a dataset containing 438 attributes, encompassing chemical compositions (e.g., carbon, silicon, manganese), heat treatment parameters (e.g., normalizing and tempering temperatures, carburizing time), and microstructural properties like inclusion area fractions. The model achieved a high R² value of 0.9892 and a Mean Squared Error (MSE) of 442.45, confirming its accuracy and robustness in predicting fatigue strength. The prediction workflow is supported by K-Nearest Neighbours (KNN) imputation to intelligently fill in missing data and Standard Scaler to ensure equal feature contribution.

The system enables users—such as engineers and researchers—to input known material parameters via a GUI or file upload interface. It then preprocesses the data, imputes missing values, and predicts the fatigue strength using the trained Gradient Boosting model. This flexibility allows for accurate predictions even when input data is incomplete. In one prediction instance, a fatigue strength of 443.73 (10⁷ cycles) was predicted using partial data, demonstrating the model's reliability. Comparative training was also conducted with other regression models like XGBoost, Random Forest, and Linear Regression, but Gradient Boosting showed superior performance across all validation metrics. The imputation strategy ensures that the model remains effective in real-world applications where complete datasets are often unavailable.

This machine learning-based system stands out for its accuracy, adaptability, and user-friendly design. By combining explainable AI, robust data preprocessing, and advanced regression techniques, it supports data-driven decisions in material selection and fatigue life assessment. The system is particularly beneficial for critical applications in aerospace, automotive, and structural engineering, where fatigue resistance is a key performance metric. Through continuous updates and feedback integration, the model evolves with new data, making it a sustainable and intelligent solution for fatigue strength prediction.

Table 1- Comparison table between the Gradient Boosting, XGBoost, Random Forest, and Linear Regression Models using MSE and R² parameters.

MSE	R ² Score	Algorithm	
442.456438	0.989298	Gradient Boosting	
544.094299	0.986840	XGBoost	
635.681707	0.984625	Random Forest	
1034.364634	0.974982	Linear Regression	

The Mean Squared error(MSE) which measures the average squared difference between the actual and predicted values is given by,

$$\mathbf{MSE} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \tag{1}$$

Where:

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n = number of data points \hat{y}_l = predicted value
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 y_i = actual value

Coefficient of Determination (R²) measures how well the regression model explains the variance in the data. This is given by,

$\mathbf{R}^{2} = 1 - \frac{\sum_{i=1}^{n} (y_{i} - \hat{y}_{i})^{2}}{\sum_{i=1}^{n} (y_{i} - \bar{y})^{2}}$	(2)	
Where:		
y_i = actual value		\overline{y} = mean of actual values
$\widehat{y}_i =$ predicted value		n = number of data points

5.1 Model Output and Interpretation

The fatigue strength prediction model developed in this project utilizes machine learning algorithms to estimate the rotating bending fatigue strength of materials based on user-supplied input parameters. Users are prompted to enter various material properties, including chemical composition (e.g., carbon, manganese, silicon), heat treatment conditions (e.g., tempering time, normalizing temperature), and microstructural features such as inclusion area fractions. The system is designed to handle incomplete user inputs through the implementation of K-Nearest Neighbours (KNN) imputation, which

intelligently approximates missing values by analysing patterns and similarities within the dataset. This capability ensures that the model maintains predictive accuracy even when certain critical parameters are unavailable.

The model's performance is inherently tied to the completeness and reliability of the input data. Alloying elements like manganese and silicon have been observed to significantly influence fatigue behaviour, highlighting the importance of accurate material data. However, the integration of imputation techniques allows the model to function reliably even under conditions of data scarcity, broadening its applicability in practical engineering contexts. This flexibility makes the system a robust and practical tool for engineers and materials scientists aiming to evaluate fatigue performance in diverse real-world scenarios, including those encountered in aerospace, automotive, and structural applications.



Fig. 3 – Graphical Representation of R² for various ML models considered

5.2 Results

The model for predicting fatigue strength is found to have a very high accuracy, with an R^2 value of 0.9892 while using Gradient boosting. This means that the model can explain about 98% of the variability in fatigue strength using the features used as inputs. It is exceptional to have such an R^2 value in predictive modelling, implying that the model is able to capture the relations between material properties and fatigue strength.

Enter material properties (leave blank if unknown):			
Enter the value for NT: 845			
Enter the value for THT: 845			
Enter the value for THt: 30			
Enter the value for THQCr: 24			
Enter the value for CT: 30			
Enter the value for Ct: 0			
Enter the value for DT:			
Enter the value for Dt:			
Enter the value for QmT:			
Enter the value for TT: 600			
Enter the value for Tt: 60			
Enter the value for TCr: 24			
Enter the value for C: .45			
Enter the value for Si: .22			
Enter the value for Mn: .72			
Enter the value for P: .011			
Enter the value for S: .025			
Enter the value for Ni: .12			
Enter the value for Cr: .12			
Enter the value for Cu: .04			
Enter the value for Mo: .13			
Enter the value for RedRatio: Ø			
Enter the value for dA:			
Enter the value for dB:			
Enter the value for dC:			
Missing features: 6 / 25			
引 Closest matching actual fatigue value: 707.00 (×10 ⁷ Cycles)			
Y Predicted fatigue strength: 443.73 (x107 Cycles)			

Fig. 4 – Output from the model

The above Fig.4 displays the final predicted fatigue output from the user input data. In real-world use, the model can accommodate users to enter different material parameters, such as chemical compositions and processing conditions. Even when partial inputs are missing, the model uses methods such as K-Nearest Neighbours (KNN) imputation to fill in missing values, making predictions still possible with a high level of confidence.

6. Conclusion and Future Scope

6.1 Conclusion

The fatigue strength prediction project summarizes that the Gradient Boosting regression model provides the best performance in rotating bending fatigue strength estimation among the models evaluated. With a high R² score of 0.9892 and minimal mean squared error, the Gradient Boosting model successfully models the intricate, non-linear interactions between material properties and fatigue strength. Its ensemble learning methodology improves generalizability and resists overfitting, rendering it a stable option for this use. The model is designed to be able to accommodate user-specified inputs so that fatigue strength prediction is possible even when certain material parameters are unknown. Using K-Nearest Neighbours (KNN) imputation, the system calculates missing values according to similarities with available data to make predictions in a reliable manner. This level of flexibility renders the model suitable for real-life applications where total data might not always be readily available. The combination of Gradient Boosting regression with smart data processing methods yields a very accurate and easy-to-use tool for fatigue strength prediction, which supports engineers and material scientists in material selection and design tasks.

6.2 Future Scope

The future potential of the fatigue strength prediction model is vast, with a number of promising avenues for development. Incorporating more materials, such as polymers, composites, and ceramics, can broaden the model's use across industries like aerospace, automotive, and construction. The use of realtime sensor and production data could facilitate dynamic and context-dependent material selection, making the model more responsive to operating conditions. Improving the model's natural language processing to understand more complicated and vague user requests would enhance its flexibility and usability. Integration with predictive maintenance systems can enable the evaluation of long-term material performance by integrating operational data with material predictions. Utilizing multi-objective optimization algorithms that take factors such as cost, sustainability, and environmental impact into consideration can create more balanced and comprehensive material selection choices. Creating industry-specific versions of the model can make it give targeted suggestions, enhancing its relevance and usability

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