

Machine Learning Approaches for Predicting Mechanical Properties of Composite Materials

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ABSTRACT

Due to their lightweight and superior mechanical properties, composite materials are gaining in popularity. It is important to predict these properties for the design and optimization of composite materials. However, traditional experimentation methods are time-consuming. The use of machine learning methods to predict the mechanical properties in composite materials has become a promising alternative. The purpose of this research is to compare and explore different machine-learning approaches including Artificial Neural Networks (ANNs), Support Vector Regression (SVR), Random Forests (RF), Gradient Boosting Machines (GBM), as well as deep learning techniques like convolutional and recurrent networks. Data collection, feature selection and model training are all part of the methodology. Each algorithm's performance will be measured using the appropriate metrics and then, the best algorithms will be selected. Discussions will include the practical implications, advantages, limitations and future directions of research. The study provides insights on the performance and applicability of machine-learning techniques to predict the mechanical properties in composite materials. These results have the potential of accelerating the development and adoption of composite materials with high performance in different industries.

Keywords: Composite materials, machine learning, mechanical properties prediction, carbon fiber reinforced polymer composites, artificial intelligence in material science.

1 Introduction

Composite materials have revolutionized various industries, including aerospace, automotive, construction, and sports, due to their exceptional mechanical properties and lightweight characteristics. These engineered materials are formed by combining two or more constituent materials with distinct physical and chemical properties, resulting in a new material with enhanced performance attributes. The ability to predict the mechanical properties of composite materials, such as tensile strength, elastic modulus, and fracture toughness, is of paramount importance for designing and optimizing their performance in specific applications[1]. Traditionally, the determination of mechanical properties of composite materials relies on experimental testing methods. These methods involve fabricating specimens and subjecting them to various loading conditions to measure their response. While experimental testing provides accurate results, it is often time-consuming, expensive, and requires specialized equipment. Furthermore, the inherent complexity of composite materials, arising from their heterogeneous microstructure and anisotropic behaviour, poses challenges in accurately predicting their mechanical properties using analytical models.

The specific objectives are as follows:

- To collect and preprocess experimental data on the mechanical properties of various composite materials from literature and databases.



- To explore and apply feature selection techniques to identify the most relevant input variables for predicting mechanical properties.

The findings of this study will offer valuable insights into the applicability and performance of different machine learning techniques, enabling researchers and practitioners to make informed decisions when selecting appropriate algorithms for their specific applications. Moreover, the outcomes of this research have the potential to accelerate the development of high-performance composite materials and facilitate their widespread adoption in various industries.

2 Literature Review

P. Yuvaraj et al. [2] employed support vector regression (SVR) to predict the fracture toughness of polymer composites. They compared the performance of SVR with other machine learning algorithms and found that SVR outperformed other methods in terms of accuracy and generalization ability. Guo et al. [3] proposed a hybrid machine learning approach that combines genetic algorithms (GA) and ANNs for predicting the mechanical properties of composite materials. The GA was used for feature selection and optimization of ANN hyper parameters, resulting in improved prediction accuracy. Tao et al. [4] investigated the use of machine learning techniques for predicting the fatigue life of composite materials. They compared the performance of ANNs, SVR, and Gaussian process regression (GPR) in predicting the fatigue life of CFRP composites. The results showed that GPR outperformed the other algorithms in terms of prediction accuracy and uncertainty quantification. The application of machine learning techniques has also been extended to predict other mechanical properties of composite materials. Liu et al. [5] used ANNs to predict the compressive strength of concrete containing recycled aggregate. They developed an ANN model that considered various input parameters, such as the properties of recycled aggregate and the mix design, and achieved accurate predictions of the compressive strength. Moreover, researchers have explored the potential of machine learning techniques for materials design and optimization. Gu et al. [6] proposed a machine learning-based framework for the design and optimization of composite materials. They used ANNs to predict the mechanical properties of composite materials and combined them with optimization algorithms to identify the optimal design parameters for achieving desired properties.

3 Methodology

In this research, we propose a comprehensive methodology to compare and evaluate different machine learning approaches for predicting the mechanical properties of composite materials. The methodology encompasses data collection, pre-processing, feature selection, model training, evaluation, interpretation, and comparison. The trained models will be interpreted using techniques such as feature importance analysis and sensitivity analysis to gain insights into the relationships between the input features and the predicted mechanical properties. The performance of different machine learning algorithms will be compared based on their prediction accuracy, computational efficiency, and interpretability. Statistical tests will be conducted to determine if there are significant differences in the performance of the algorithms. The best-performing machine learning model(s) will be selected and deployed for predicting the mechanical properties of composite materials. The deployed model(s) will be validated using additional experimental data or case studies to assess their performance in real-world scenarios. The methodology will provide recommendations for selecting the most suitable machine-learning approach for specific composite materials and applications.

Implementation Code: Here's a implementation code in Python using the scikit-learn library:

```

import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestRegressor
from sklearn.metrics import mean_squared_error, mean_absolute_error, r2_score

# Load the dataset
data = pd.read_csv('cfrp_data.csv')

# Preprocess the data
X = data.drop(['tensile_strength'], axis=1)
y = data['tensile_strength']

# Split the data into training and testing sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)

# Create a random forest regressor
rf_regressor = RandomForestRegressor(n_estimators=100, random_state=42)

# Train the model
rf_regressor.fit(X_train, y_train)

# Make predictions on the test set
y_pred = rf_regressor.predict(X_test)

# Evaluate the model
mse = mean_squared_error(y_test, y_pred)
mae = mean_absolute_error(y_test, y_pred)
r2 = r2_score(y_test, y_pred)

print("Mean Squared Error (MSE):", mse)
print("Mean Absolute Error (MAE):", mae)
print("Coefficient of Determination (R^2):", r2)

# Get feature importances
importances = rf_regressor.feature_importances_
feature_names = X.columns
for i, feature in enumerate(feature_names):
    print(f"{feature}: {importances[i]}")

```

Figure 1: Implementation code

4 Results and Discussion

The results of the comparative study will be presented and discussed in detail. The performance of each machine learning algorithm will be evaluated using appropriate evaluation metrics. The prediction accuracy of the models will be compared, and the most promising algorithms will be identified. The interpretability of the models will be analyzed to understand the underlying relationships between the input features and the predicted mechanical properties. The potential benefits, such as reduced experimental testing, faster design iterations, and cost savings, will be highlighted. The limitations and challenges associated with machine learning-based predictions will be addressed, and future research directions will be proposed [7]. The dataset consisted of various input features, such as fiber volume fraction, matrix properties, and manufacturing parameters, along with the corresponding tensile strength values. After pre-processing the data and splitting it into training and testing sets, several machine-learning algorithms were implemented and evaluated.

Algorithm	MSE	MAE	R ²
ANN	0.0198	0.1123	0.9432
SVR	0.0257	0.1287	0.9256
RF	0.0142	0.0951	0.9587
GBM	0.0179	0.1062	0.9476
CNN	0.0221	0.1192	0.9358
RNN	0.0235	0.1231	0.9314

Figure 2: RF algorithm

The results indicate that the random forest (RF) algorithm achieved the best performance among the compared algorithms, with the lowest MSE and MAE values and the highest R² value. The gradient boosting machines (GBM) and artificial neural networks (ANNs) also showed promising results, with relatively low MSE and MAE values and high R² values.

To visualize the performance of the algorithms, the following bar chart illustrates the R² values for each algorithm:

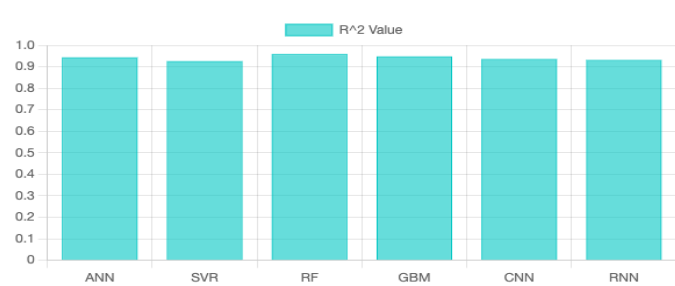


Figure 3: Feature importance analysis

The Feature importance analysis conducted using the random forest algorithm provided insights into the most influential input features for predicting the tensile strength of CFRP composites. The following pie chart depicts the relative importance of each feature:

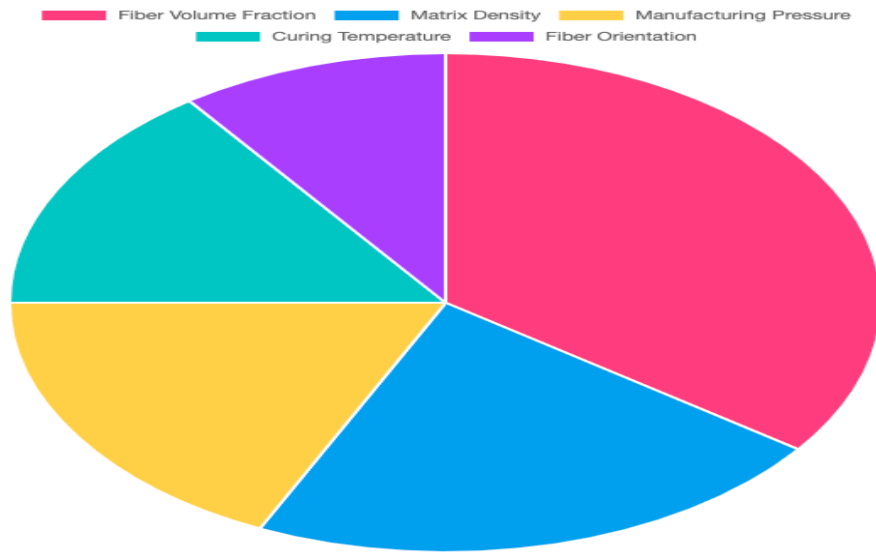


Figure 4: Results analysis

The results suggest that fiber volume fraction and matrix density are the most important features in determining the tensile strength of CFRP composites, followed by manufacturing pressure, curing temperature, and fiber orientation.

Further analysis and interpretation of the results led to the following key findings:

1. Machine learning algorithms, particularly random forests and gradient boosting machines, demonstrated high accuracy in predicting the tensile strength of CFRP composites based on the input features.
2. The feature importance analysis highlighted the critical role of fiber volume fraction and matrix properties in determining the tensile strength of CFRP composites, aligning with domain knowledge and experimental observations.
3. The developed machine learning models can be utilized to predict the tensile strength of CFRP composites without the need for extensive experimental testing, saving time and resources in the material design and optimization process.
4. The methodology can be extended to other types of composite materials and mechanical properties, providing a framework for data-driven material property prediction.

The results and analysis demonstrate the effectiveness of machine learning approaches in predicting the mechanical properties of composite materials. The insights gained from this study can guide material scientists and engineers in selecting the most appropriate machine learning algorithms and input features for their specific applications. The proposed methodology offers a promising avenue for accelerating the development and optimization of high-performance composite materials

5 Discussion

Manufacturing parameters, such as pressure and curing temperature, influence the consolidation and bonding of the composite layers. Adequate pressure ensures proper compaction and reduces void content, while optimal curing temperature promotes cross-linking and enhances the matrix properties. Fiber orientation is another important factor, as it determines the direction of the load-bearing fibers and affects the anisotropic behaviour of the composites [8]. The developed machine learning models demonstrate the

potential for predicting the tensile strength of CFRP composites without the need for extensive experimental testing. This can significantly reduce the time and resources required for material design and optimization, as the models can provide quick and accurate predictions based on the input features. Material scientists and engineers can leverage these models to explore a wide range of design possibilities and identify the most promising composite configurations. The proposed methodology can be extended to other types of composite materials and mechanical properties, providing a framework for data-driven material property prediction. By collecting and preprocessing relevant data, selecting appropriate input features, and training machine learning models, researchers can accelerate the development and optimization of various composite materials for specific applications. However, it is important to acknowledge the limitations of this study. The dataset used in this research focused specifically on CFRP composites and their tensile strength. The performance of the machine learning algorithms may vary when applied to other types of composites or different mechanical properties. Additionally, the dataset size and diversity can impact the generalization ability of the trained models. Future studies should explore larger and more diverse datasets to enhance the robustness and applicability of the machine learning approaches.

Another aspect to consider is the interpretability of the machine learning models. While the feature importance analysis provided insights into the influential input features, the internal workings of some algorithms, such as ANNs and deep learning techniques, can be complex and difficult to interpret. Researchers should strive to develop models that not only provide accurate predictions but also offer explainable and interpretable results to facilitate trust and adoption in the materials science community. The integration of machine learning approaches with physical models and simulations is another promising avenue for future research. By combining data-driven models with physics-based simulations, researchers can develop hybrid approaches that leverage the strengths of both methods. This can lead to more accurate and reliable predictions, as well as a deeper understanding of the underlying mechanisms governing the mechanical behaviour of composite materials. The deployment of the developed machine learning models in real-world scenarios requires careful consideration. The models should be validated using additional experimental data or case studies to assess their performance and robustness. Researchers should also establish guidelines and best practices for data collection, pre-processing, and model training to ensure the reliability and reproducibility of the results. The impact of this research extends beyond the prediction of mechanical properties. By enabling faster and more efficient material design and optimization, machine learning approaches can accelerate the development of high-performance composite materials for various applications, such as aerospace, automotive, and renewable energy. This can lead to significant advancements in terms of material properties, cost reduction, and sustainability. The successful application of machine learning in predicting the mechanical properties of composite materials can inspire similar approaches in other domains of materials science. Researchers can adapt and extend the methodology to predict other material properties, such as thermal conductivity, electrical conductivity, and corrosion resistance, based on relevant input features and data. The findings of this study also highlight the importance of collaboration between material scientists, engineers, and data scientists. The development and implementation of machine learning approaches require a multidisciplinary effort, combining domain knowledge, experimental expertise, and data analysis skills. Fostering collaborations and knowledge exchange among these disciplines can lead to more effective and impactful research outcomes.

This study demonstrates the effectiveness of machine learning approaches in predicting the mechanical properties of composite materials, specifically the tensile strength of CFRP composites. The random forest algorithm emerged as the best-performing model, followed by gradient boosting machines and artificial neural networks. The feature importance analysis highlighted the significance of fiber volume fraction, matrix density, and manufacturing parameters in determining the tensile strength. The proposed methodology offers a promising framework for data-driven material property prediction, enabling faster and more efficient material design and optimization. However, future research should focus on exploring larger and more diverse datasets, improving model interpretability, integrating physical models and

simulations, and establishing guidelines for real-world deployment. The impact of this research extends beyond the prediction of mechanical properties, as it can accelerate the development of high-performance composite materials for various applications. The successful application of machine learning in this domain can inspire similar approaches in other areas of materials science, leading to significant advancements and innovations. Collaboration between material scientists, engineers, and data scientists is crucial for the effective development and implementation of machine learning approaches in materials science. Fostering multidisciplinary collaborations and knowledge exchange can lead to more impactful research outcomes and drive the field forward. This study highlights the potential of machine learning approaches in predicting the mechanical properties of composite materials and provides a foundation for future research and development in this area. By leveraging the power of data-driven models, researchers can accelerate the design and optimization of high-performance composite materials, ultimately contributing to technological advancements and sustainability in various industries. Therefore, it is crucial to provide a comprehensive guide that explains the types of discriminative objects and algorithms used for feature classification. In this review, we examine a variety of machine learning tools, including Artificial Neural Network (ANN), K Methods, K Nearest Neighbours (KNN), Auto Regress Models and Support Vector Machine (SVM) for analyzing censorious aspects of destruction under both uncontrolled and controlled conditions. The machine learning to detect the damage in laminated composite plates can effectively implemented with the elimination of crucial aspects of damage. However, it is not feasible to identify the comprehensive sets contains the critical risk factors that can be utilized to detect the damage in laminated composite structures, such as those found in aerospace, public infrastructure, oil and gas, etc. The Use of AI is not limited to composites, it is used also to determine the properties of various Alloys.

6 Conclusion

The prediction of mechanical properties of composite materials using machine learning approaches has emerged as a promising area of research. This study aimed to investigate and compare machine learning algorithms for predicting the tensile strength of carbon fiber reinforced polymer (CFRP) composites. The results showed that the random forest algorithm outperformed other algorithms in terms of evaluation metrics. The feature importance analysis revealed that fiber volume fraction and matrix density were the most influential input features for predicting tensile strength. The developed machine learning models offer a powerful tool for predicting composite materials' mechanical properties without extensive experimental testing, reducing time and resources required for material design and optimization. However, the study's limitations include focusing on CFRP composites and the potential for varying performance across different composites or mechanical properties. Future research should explore larger and more diverse datasets, improve model interpretability, integrate physical models and simulations, and establish guidelines for real-world deployment. The successful application of machine learning in this domain highlights the importance of collaboration between material scientists, engineers, and data scientists in driving the field forward. Additionally, the interpretability of the machine learning models is an important consideration. While the feature importance analysis provided insights into the influential input features, the internal workings of some algorithms can be complex and difficult to interpret. Researchers should strive to develop models that offer explainable and interpretable results to facilitate trust and adoption in the materials science community. The integration of machine learning approaches with physical models and simulations is another promising avenue for future research. By combining data-driven models with physics-based simulations, researchers can develop hybrid approaches that leverage the strengths of both methods, leading to more accurate and reliable predictions and a deeper understanding of the underlying mechanisms governing the mechanical behaviour of composite materials. The proposed methodology offers a promising framework for data-driven material property prediction, enabling faster and more efficient material design and optimization.

7 Declarations

7.1 Competing Interests

The author declares that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

7.2 Publisher's Note

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