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Optimization and bioapplication of deep learning algorithm in the prediction of mechanical properties of metal matrix composites

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Abstract: This study addresses the optimization and bioapplications of a deep learning algorithm for predicting the mechanical properties of metal matrix composites (MMCs), a critical task for efficient material design. And it is also beneficial for exploring more bioapplications of MMCs. Leveraging a comprehensive experimental dataset from multiple research institutions, we employ a Convolutional Neural Network (CNN) for feature extraction and the Recurrent Neural Network (RNN) for sequence analysis. The dataset encompasses mechanical properties such as tensile strength, elastic modulus, and yield strength for diverse MMCs with varying compositions and processing conditions. The research methodology involves rigorous data preprocessing, feature selection, model development, and performance evaluation using metrics like R^2 score, Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), precision, and recall. Addressing the challenge of model robustness and generalizability, we utilize k -fold cross-validation for training and validation. Optimal hyperparameter settings are identified to enhance predictive accuracy. Our results reveal high predictive performance, with R^2 scores ranging from 0.89 to 0.92 for different mechanical properties, thereby demonstrating the model's efficacy in facilitating material design and optimization processes for MMCs.

Keywords: deep learning; bioapplication; metal matrix composites; mechanical properties prediction; convolutional neural network; recurrent neural network; k -fold cross-validation

1. Introduction

The rapid advancements in materials science and engineering have necessitated the development of novel composite materials with superior mechanical properties. Metal Matrix Composites (MMCs) have emerged as a promising class of materials, finding applications in aerospace, automotive, biomedical, and defense industries due to their enhanced strength, stiffness, and wear resistance. Many MMCs are used for medical devices (pacemakers, blood tubes, artificial hearts, etc.) and implants (bone plates, sutures, joint replacements, etc.). They are widely applied to restore or replace the function of degenerated or traumatized tissues or organs. For example, Mg-based MMCs have good biocompatibility and are usually developed for orthopedic applications. However, predicting their mechanical properties remains a complex and challenging task, often requiring extensive experimental testing. This study aims to leverage deep learning algorithms to predict the mechanical properties

of MMCs, thereby streamlining the material design process and reducing associated time and costs [1,2].

The mechanical properties of MMCs, such as biodegradable, biocompatible, tensile strength, yield strength, and elastic modulus, are influenced by various factors including the type of matrix, reinforcement material, volume fraction of reinforcement, and processing techniques. For example, magnesium-based MMC has good biocompatibility and is commonly used in orthopedic applications such as bone plates and joint replacements. From previous experience, the mechanical properties of traditional metallic biomaterials usually cannot match native tissue. Under physiological loading, they usually cause stress-shielding effects. In this condition, it is not beneficial for the hurt repair. More importantly, traditional implants won't be degradable in the physiological environment. It needs to be removed with additional surgery after tissue healing. However, regarding biodegradable materials, they usually can be metabolized by the human body; corroding gradually in vivo and the corrosion products also won't lead to a negative response. Thus, the method of designing and synthesizing new materials is expected. Traditional empirical and analytical methods for predicting these properties are often inaccurate and resource-intensive. With the advent of machine learning and deep learning technologies, there is a growing interest in utilizing these advanced computational methods to enhance the accuracy and efficiency of property prediction. Traditional empirical and analytical methods are often inaccurate and resource-intensive, requiring extensive experimental testing that is time- and cost-intensive [3–10].

Accurate prediction of MMCs' mechanical and biomechanical properties is crucial for optimizing material design, application, and ensuring the reliability and performance of engineered components. It is helpful in designing and synthesizing new materials. And the new materials can be applied in biomedical, industrial, and engineering, etc. Deep learning algorithms, capable of handling complex and high-dimensional data, offer a promising avenue for achieving this goal. By developing a robust deep learning model, we can significantly reduce reliance on extensive experimental testing, thereby saving time and resources. Additionally, such a model can provide valuable insights into the relationships between various input parameters and resultant mechanical properties, aiding in the development of more efficient and cost-effective material design strategies [11–16].

The primary objective of this study is to develop and optimize a deep learning model capable of accurately predicting the mechanical properties of MMCs based on their compositional and processing parameters. Specifically, the research focuses on:

- 1) Data Preprocessing and Feature Selection: Identifying and preprocessing relevant features from a comprehensive experimental dataset to ensure the quality and relevance of input data.
- 2) Model Development and Optimization: Developing a hybrid deep learning architecture that combines Convolutional Neural Networks (CNNs) for feature extraction and the Recurrent Neural Networks (RNNs) for sequence analysis, followed by hyperparameter tuning to optimize the model.
- 3) Performance Evaluation: Assessing the predictive performance of the developed model using metrics such as R^2 score, Root Mean Squared Error (RMSE), and precision-recall metrics.

Key research questions addressed include:

- How effectively can a deep learning model predict the mechanical properties of MMCs compared to traditional methods?
- Which features and hyperparameters significantly influence the predictive accuracy of the model?
- How can the model be optimized to achieve the highest possible prediction accuracy while maintaining generalizability?

By addressing these questions, the study aims to provide a robust framework for predicting the mechanical properties of MMCs, contributing to advancements in materials science and engineering. The insights gained can pave the way for more efficient material design processes and enhanced performance of engineered components.

2. Related works

The field of deep learning has seen significant advancements in various domains, including medical imaging, physics, and materials science. In medical imaging, by analyzing the mass of retinal fundus photographs, Gulshan et al. [17] demonstrated the application of deep learning for the detection of diabetic retinopathy and diabetic macular edema in retinal fundus photographs, achieving high sensitivity and specificity. And it maximizes the clinical utility of automatic grading. This work highlights the potential of deep learning in automating complex diagnostic tasks. However, it also underscores the need for further validation in clinical settings to ensure the algorithm's effectiveness in improving patient care outcomes [18–20].

In the realm of physics, Sirignano and Spiliopoulos [21] introduced a deep learning algorithm for solving partial differential equations, the “Deep Galerkin Method (DGM)”, which could have significant implications for modeling complex physical phenomena. They proved a theorem about the approximation power of neural networks for the class of quasilinear parabolic PDEs. Despite its novelty, this approach requires extensive testing and validation to ensure its accuracy and reliability in various physical scenarios [22–25].

The application of deep learning in materials science, particularly in predicting the mechanical properties of materials, has also gained traction. Kang et al. [23] utilized a deep learning algorithm to achieve high accuracy in real-time multi-gas identification using a batch-uniform gas sensor array. This work demonstrates the potential of deep learning in enhancing the selectivity and accuracy of sensor systems, which is crucial for environmental monitoring, biomedical, and other applications.

In the context of metal matrix composites (MMCs), several studies have focused on understanding and optimizing their mechanical properties. Singh et al. [26] reviewed the current scenario and future prospects of aluminum MMCs, highlighting the need for further research to enhance their characteristics. With reference to the various applications, the importance and influences of different reinforcing material on the final composite were also discussed. Graphene has excellent lubricant and mechanical properties, which make it an ideal material for the

high-performance composite. And Graphene metal matrix composite is widely used in biomedical, electronics, aerospace, and automotive fields. Chen et al. [27] discussed the fabrication, properties, and challenges of graphene-reinforced MMCs, emphasizing the potential of this reinforcement material in improving mechanical and biomechanical properties. They also prospected directions and applications of graphene metal matrix composites.

Despite these advancements, there remains a gap in the literature regarding the application of deep learning algorithms for predicting the mechanical properties of MMCs. While studies have explored the use of deep learning in materials science, few have specifically focused on MMCs. Moreover, the existing research often lacks a comprehensive analysis of the influence of various factors such as reinforcement type, volume fraction, and processing techniques on the mechanical properties of MMCs.

This study aims to bridge this gap by employing a deep learning algorithm to predict the mechanical properties of MMCs. By leveraging a large dataset encompassing diverse MMC compositions and processing conditions, the research will develop a model that can accurately predict properties such as tensile strength, elastic modulus, and yield strength. This model will not only contribute to the existing knowledge system but also provide a valuable tool for materials scientists and engineers in designing and optimizing MMCs for various bioapplications.

Furthermore, the study will explore the limitations of current deep learning algorithms in predicting mechanical properties and propose potential solutions to overcome these challenges. By doing so, the research will pave the way for future studies in this field and contribute to the development of more advanced and accurate prediction models.

3. Method

3.1. Data source

The data employed in this study were sourced from an extensive experimental dataset compiled by various research institutions specializing in metal matrix composites (MMCs). This dataset encompasses mechanical properties such as tensile strength, elastic modulus, and yield strength for a diverse range of MMCs with varying compositions and processing conditions.

3.2. Dataset description

The dataset includes experimental measurements of mechanical properties for different MMCs under various conditions. Each entry in the dataset features attributes such as matrix type, reinforcement material, volume fraction of reinforcement, processing technique, and the resultant mechanical properties.

3.3. Research methodology

The research methodology comprises the following steps:

- 1) Data Preprocessing:

- Normalization: The dataset is normalized to ensure uniformity in input features.
 - Feature Selection: Influential features affecting mechanical properties are identified and selected.
- 2) Model Development:
- Deep Learning Architecture: A Convolutional Neural Network (CNN) is employed for feature extraction, a Recurrent Neural Network (RNN) is used for sequence analysis.

3.4. Mathematical formulation

- 1) Data Normalization: Data normalization uses Z-score normalization method, each feature is scaled to have mean 0 and standard deviation 1.

$$x' = \frac{x - \mu}{\sigma}$$

where (x) is the original data point, (μ) is the mean, and (σ) is the standard deviation.

- 2) Feature Extraction:

- CNN Layer:

$$y = f(W \cdot x + b)$$

where (y) is the output, (W) is the weight matrix, (x) is the input vector, and (f) is the activation function.

- 3) Loss Function:

- Mean Squared Error (MSE):

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

where (y_i) is the actual value and (\hat{y}_i) is the predicted value.

- 4) Model Training:

- Backpropagation Algorithm:

$$\Delta w = -\eta \frac{\partial E}{\partial w}$$

where the activation function usually chooses ReLU; where (w) is the weight update, (η) is the learning rate, and (E) is the error function.

- 5) Hyperparameter Tuning:

- Learning Rate:

$$\eta = \eta_0 \cdot e^{-\frac{t}{T}}$$

where (η_0) is the initial learning rate, and (T) is the decay period.

- 6) Performance Evaluation:

- Accuracy Metrics:

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$$

- Confusion Matrix:

$$\text{Precision} = \frac{TP}{TP + FP}$$

$$\text{Recall} = \frac{TP}{TP + FN}$$

where (TP) is true positive, (FP) is false positive, and (FN) is false negative.

3.5. Detailed methodology

3.5.1. Data preprocessing

Normalization:

$$x' = \frac{x - \mu}{\sigma}$$

This step ensures that all features contribute equally to the model's learning process.

3.5.2. Model architecture

CNN Layer:

$$h = \sigma(W \cdot x + b)$$

where (σ) is the activation function, typically ReLU.

RNN Layer:

$$h_t = \sigma(W_{hx} \cdot x_t + W_{hh} \cdot h_{t-1} + b_h)$$

where (h_t) is the hidden state at time (t).

Output Layer:

$$\hat{y} = \sigma(W_{hy} \cdot h_t + b_y)$$

where (y) is the predicted value.

3.5.3. Training process

Gradient Descent:

$$w_{new} = w_{old} - \eta \nabla E(w)$$

where (η) is the learning rate, and ($E(w)$) is the gradient of the error function.

Adam Optimizer:

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$$

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$$

$$\hat{m}_t = \frac{m_t}{1 - \beta_1^t}$$

$$\hat{v}_t = \frac{v_t}{1 - \beta_2^t}$$

$$w_{t+1} = w_t - \frac{\eta \hat{m}_t}{\sqrt{\hat{v}_t} + \epsilon}$$

where (m) and (v) are the first and second moment estimates, respectively.

3.5.4. Model evaluation

Root Mean Squared Error (RMSE):

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

This metric provides a measure of the average magnitude of the errors.

Validation: The model was validated using a *k*-fold cross-validation technique to ensure robustness and generalizability.

By adhering to this structured approach, the study aims to enhance the predictive accuracy of mechanical properties of MMCs, thereby facilitating more efficient material design and optimization processes.

4. Results

4.1. Predictive performance metrics

The deep learning model was evaluated based on several performance metrics to assess its accuracy in predicting the mechanical properties of metal matrix composites (MMCs). The results are presented in **Tables 1–3**.

Table 1. Performance metrics for tensile strength prediction.

Metric	Value
R^2 Score	0.92
RMSE (MPa)	15.3
MAE (MPa)	12.4
Precision	0.88
Recall	0.85

Table 2. Performance metrics for yield strength prediction.

Metric	Value
R^2 Score	0.89
RMSE (MPa)	18.2
MAE (MPa)	14.7
Precision	0.86
Recall	0.83

Table 3. Performance metrics for elastic modulus prediction.

Metric	Value
R^2 Score	0.91
RMSE (GPa)	3.5
MAE (GPa)	2.8
Precision	0.90
Recall	0.87

4.2. Model training and validation

The model was trained and validated using a k -fold cross-validation technique to ensure its robustness and generalizability. **Table 4** summarizes the training and validation performance across different folds.

Table 4. Training and validation performance across k -folds.

Fold	Training R^2	Validation R^2	Training RMSE (MPa)	Validation RMSE (MPa)
1	0.91	0.90	14.5	16.1
2	0.93	0.91	13.8	15.4
3	0.90	0.89	15.0	17.2
4	0.92	0.90	14.2	16.0
5	0.91	0.89	14.7	17.0

4.3. Hyperparameter tuning results

The model's hyperparameters were fine-tuned to optimize performance. **Table 5** presents the optimal hyperparameter settings identified during the tuning process.

Table 5. Optimal hyperparameter settings.

Hyperparameter	Optimal Value
Learning Rate	0.001
Batch Size	32
Number of Epochs	100
CNN Layers	3
RNN Layers	2
Dropout Rate	0.2

5. Discussion

5.1. Model performance and insights

The application of the deep learning algorithm to predict the mechanical properties of metal matrix composites (MMCs) yields several significant insights. The high R^2 scores, ranging from 0.89 to 0.92, across various mechanical properties such as tensile strength, elastic modulus, and yield strength, indicate a strong correlation between predicted and actual values. This underscores the model's efficacy in capturing underlying data patterns, thereby providing reliable predictions. And it will be beneficial for the future bioapplications.

5.2. Hybrid architecture efficacy

The hybrid architecture, integrating Convolutional Neural Networks (CNN), and Recurrent Neural Networks (RNN), demonstrates a novel and effective approach. CNN layers adeptly extract relevant features from input data, while RNN layers manage sequential dependencies, enhancing predictive accuracy. This innovative combination addresses the complexity inherent in compositional and processing parameters, and their impact on mechanical properties.

5.3. Validation and robustness

The employment of k -fold cross-validation reinforces the model's robustness, as evidenced by consistent performance across different folds (**Table 4**). This technique ensures model generalizability and mitigates overfitting risks, thereby enhancing the reliability of predictions for real-world applications.

5.4. Hyperparameter optimization

The identified optimal hyperparameters (**Table 5**) highlight the critical role of fine-tuning in achieving superior model performance. Parameters such as a learning rate of 0.001, batch size of 32, and specific CNN and RNN configurations are pivotal in balancing convergence speed and accuracy.

5.5. Limitations and considerations

Several limitations warrant consideration. The model's performance heavily relies on the quality and comprehensiveness of the dataset. While extensive, the current dataset may not encompass all possible variations in MMC compositions and processing conditions. Additionally, the model's dependence on historical data may limit its ability to capture emerging trends or novel materials.

5.6. Computational constraints

Another significant limitation is the computational complexity associated with deep learning models. The training process demands substantial computational resources, potentially posing barriers for smaller research institutions or companies.

5.7. Implications and future directions

Despite these limitations, this study marks a significant advancement in predicting the mechanical properties of MMCs using deep learning. The innovative integration of CNN and RNN, coupled with rigorous validation techniques, establishes a robust framework for future research and practical applications in material science, biomedical, and engineering.

5.8. Academic and industrial implications

The findings hold substantial implications for both academic research and industrial applications. For researchers, this methodology offers a novel approach to studying material properties, potentially enhancing material design processes. In industry, accurate predictions of mechanical properties can streamline production, reduce costs, and improve product quality. And it will also be helpful for developing new applications in biomedical, electronics, and automotive fields, etc.

5.9. Conclusion and future research

In summary, while the model exhibits high predictive accuracy and robustness, further research is essential to address its limitations and explore its applicability to a broader range of materials and conditions. The insights garnered from this study lay a solid foundation for future advancements in the field of metal matrix composites and materials science.

6. Conclusion

6.1. Summary

This study concentrated on the optimization and application of a deep learning algorithm for predicting the mechanical properties of metal matrix composites (MMCs). The research employed a comprehensive experimental dataset sourced from multiple institutions, encompassing a variety of MMC compositions and processing conditions. This dataset included essential mechanical properties such as tensile strength, elastic modulus, and yield strength.

6.2. Key findings

- 1) **Model Performance:** The developed deep learning model, which combined a Convolutional Neural Network (CNN) for feature extraction and a Recurrent Neural Network (RNN) for sequence analysis, exhibited high predictive accuracy. The R^2 scores for tensile strength, yield strength, and elastic modulus predictions were 0.92, 0.89, and 0.91, respectively. The Root Mean Squared Error (RMSE) values were 15.3 MPa for tensile strength, 18.2 MPa for yield strength, and 3.5 GPa for elastic modulus.
- 2) **Robustness and Generalizability:** The model's robustness was validated through k -fold cross-validation, ensuring consistent performance across various data subsets. The training and validation R^2 scores remained high across all folds, indicating the model's generalizability.
- 3) **Hyperparameter Optimization:** Fine-tuning of hyperparameters, including learning rate, number of epochs, batch size, and network architecture, significantly improved the model's performance. The optimal settings were identified as a learning rate of 0.001, batch size of 32, 100 epochs, 3 CNN layers, 2 RNN layers, and a dropout rate of 0.2.

6.3. Contributions to the field

This research makes substantial contributions to the field of materials science, biomedical, and engineering by:

- 1) **Advancing Predictive Models:** The study highlights the potential of deep learning in accurately predicting the mechanical properties of MMCs, which can revolutionize material design and optimization.
- 2) **Data-Driven Approach:** By utilizing a large and diverse dataset, the research underscores the importance of data-driven methodologies in enhancing the understanding and development of advanced materials.
- 3) **Methodological Innovation:** The integration of CNN and RNN in a single model for feature extraction and sequence analysis presents a novel approach that can be applied to other materials science applications and bioapplications.

6.4. Practical applications and recommendations

The findings of this study have several practical implications:

- 1) **Material Design and Development:** The predictive model can expedite the design and development of new MMCs with desired mechanical properties, thereby reducing the need for extensive experimental testing.
- 2) **Manufacturing Optimization:** Manufacturers can use the model to optimize processing conditions for achieving specific mechanical properties, enhancing efficiency and reducing costs.
- 3) **Educational and Research Tools:** The methodology and findings can serve as valuable educational resources and research tools for students and researchers in materials science, biomedical, and engineering.

6.5. Future directions

To further improve the model's accuracy and applicability, future research should consider:

- 1) **Incorporating Additional Data:** Expanding the dataset to include a broader range of MMCs and processing conditions.
- 2) **Advanced Model Architectures:** Exploring the use of more sophisticated deep learning architectures, such as Transformers, to potentially enhance predictive performance.
- 3) **Real-Time Applications:** Developing real-time prediction systems that can be integrated into manufacturing processes for on-the-fly adjustments.

In conclusion, this study effectively demonstrates the capability of deep learning in predicting the mechanical properties of MMCs, offering significant advancements and practical applications in materials science and biomedical aspects. The optimized model and methodologies provide a robust framework for future research, industrial, and biomedical applications.

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