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International Journal of Research Publication and Reviews

Journal homepage: www.ijrpr.com ISSN 2582-7421

Machine Learning-Based Prediction of Corrosion Behaviour in Magnesium Alloys for Biomedical Implants

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ABSTRACT

The design of magnesium-based bio-implants for bone applications demands materials with optimal mechanical properties and minimal corrosion rates to ensure biocompatibility and long-term performance. Traditional material selection methods struggle to account for the complex interplay of alloy compositions, processing techniques, and experimental conditions. This study leverages machine learning (ML) to predict the corrosion behaviour of magnesium alloys using a dataset comprising textual descriptions of materials and processing methods, numerical alloy compositions, experimental durations, corrosion rates. This study evaluates multiple ML techniques, including Random Forest, Gradient Boosting, Support Vector Regression (SVR), Neural Networks, K-Nearest Neighbours, LightGBM, and XGBoost. Textual data is pre-processed using one-hot encoding, while numerical features are normalized to enhance model accuracy. Feature selection identifies key predictors, such as alloy composition and processing conditions, optimizing the predictive framework. Results demonstrate that ML effectively correlates material attributes with performance outcomes, offering a data-driven approach to select magnesium alloys for bio-implants. This methodology outperforms conventional techniques, paving the way for advanced material optimization in biomedical engineering.

1.Introduction

The development of bio-implants has become a significant area of research in biomedical engineering, particularly in orthopaedic applications. Magnesium alloys have gained widespread attention due to their desirable properties, including lightweight structure, mechanical strength comparable to human bone, and biodegradability, which reduces the need for secondary surgeries for implant removal [1]. Despite these advantages, magnesium alloys are prone to rapid corrosion in physiological environments, which can compromise their structural integrity before the healing process is complete [2]. This challenge necessitates the identification of alloys with an optimal balance between mechanical strength and corrosion resistance.

Traditional material selection methods often rely on extensive experimental trials, requiring significant time and financial resources. Moreover, the complexity of magnesium alloys—considering factors such as alloy composition, processing methods, and environmental exposure—makes manual selection impractical [3]. Advances in machine learning (ML) provide an alternative approach, offering data-driven predictive models to streamline material selection and optimize alloy properties [4]. By analyzing large datasets containing information on alloy composition, processing techniques, and experimental conditions, ML algorithms can predict the corrosion rates and mechanical performance of various magnesium-based materials with high accuracy [5].

ML models such as including Random Forest, Gradient Boosting, Support Vector Regression (SVR), Neural Networks, K-Nearest Neighbours, LightGBM, and XGBoost have been successfully applied in materials science for property prediction. These techniques allow for better feature selection, pattern recognition, and correlation analysis between input variables and material performance outcomes [6]. Preprocessing methods, including one-hot encoding for categorical data and normalization for numerical features, enhance model performance and ensure robust predictions [7].

The integration of ML in the selection of magnesium alloys for bio-implants presents a paradigm shift from traditional trial-and-error approaches to data-driven decision-making. This study explores various ML techniques to develop a predictive framework that enables researchers and biomedical engineers to identify the most suitable magnesium alloys for bone implants efficiently. By leveraging computational techniques, the study aims to contribute to the advancement of next-generation bioresorbable implants with improved mechanical reliability and controlled degradation rates.

2.Methodology:

2.1Dataset and features:

This study collected material data from the published literature. A total of 292 different alloy compositions, a curated dataset comprising various

magnesium alloy compositions, processing techniques, and corresponding corrosion rates derived from experimental studies. The dataset includes both numerical and categorical variables, with over 40 features representing elemental composition percentages (e.g., Zn, Mn, Al, Ca), operation types, solution types, and testing methods. The corrosion rate, which is the target variable for prediction, varies in measurement, some being presented as single values while others as ranges [8][9].

2.2 Preprocessing:

Data preprocessing is a crucial step to ensure that machine learning models function optimally. Categorical variables such as operation type, solution type, and *method* were encoded using Label Encoding [10]. This transformation ensures that textual data is represented numerically while preserving the relational integrity of categories. For numerical consistency, any missing values in the dataset were replaced with 0 to avoid model bias introduced by imputation techniques [11]. This approach aligns with best practices in handling incomplete datasets in predictive modelling.

Additionally, when corrosion rates were reported as ranges (e.g., "0.2–0.4 mm/year"), they were converted into a single numeric entry by calculating the average value of the range [12]. All numerical values were then standardized using z-score normalization to ensure uniformity across features and to prevent skewed results during training [13].

2.3 Feature Selection

Given the high dimensionality of the dataset, feature selection played an essential role in reducing overfitting and improving model performance. Initially, a mutual information regression technique was applied to select the top 40 features most correlated with the corrosion rate, utilizing the Select KBest method [14]. This approach ensured that only the most relevant features were retained for training.

Further feature refinement was achieved using Recursive Feature Elimination (RFE) in combination with a Random Forest model to identify the 25 most predictive features [15]. This allowed the removal of less significant predictors, thereby improving both computational efficiency and model interpretability. Additionally, polynomial features of degree 2 were generated in an interaction-only mode, enabling the model to capture higher-order relationships between selected features [16].

2.4 Model Building and Hyperparameter Tuning

The pre-processed dataset was split into training (80%) and test (20%) sets using random shuffling. A diverse set of seven machine learning models were evaluated for their ability to predict the corrosion rates of magnesium alloys: Random Forest Regressor, Gradient Boosting Regressor, Support Vector Regressor (SVR), Multi-Layer Perceptron (Neural Networks), K-Nearest Neighbours (KNN), LightGBM, XGBoost [17][18][19]

To ensure that these models achieved optimal performance, hyperparameter tuning was conducted using GridSearchCV for the Random Forest model, optimizing estimators and maximum depth over a 5-fold cross-validation process. Other models were initialized with the best-practice hyperparameters suggested by previous studies [20][21].

2.5 Evaluation Metrics

The performance of each model was assessed using the coefficient of determination (R^2), which indicates the proportion of variance in the target variable that is explained by the model [22]. An R^2 value close to 1.0 indicates strong predictive accuracy. To provide additional context, both Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) were also computed to quantify the absolute and squared errors in the predictions [23].

These evaluation metrics are widely accepted in the field of materials science to assess the predictive power of models in both mechanical and corrosion property prediction [24][25]. The mathematical formulations for these metrics are as follows:

1. Coefficient of Determination (R^2)

$$R^2 = 1 - [\Sigma (y_i - \hat{y}_i)^2] / [\Sigma (y_i - \bar{y})^2]$$

Where:

- y_i = actual value
- $\hat{y}_i$ = predicted value
- $\bar{y}$ = mean of actual values
- n = number of data points

Explanation:

The R^2 score represents the proportion of variance in the dependent variable that is predictable from the independent variables.
A value of $R^2 = 1$ indicates perfect prediction, while $R^2 = 0$ means the model performs no better than the mean.

2. Mean Absolute Error (MAE)

$MAE = (1/n) \Sigma |y_i - \hat{y}_i|$

Explanation:
MAE measures the average magnitude of errors in a set of predictions, without considering their direction.

It is a linear score, meaning all individual differences are weighted equally in the average.

3. Root Mean Square Error (RMSE)

$RMSE = \sqrt{[(1/n) \Sigma (y_i - \hat{y}_i)^2]}$

Explanation:

RMSE penalizes large errors more than MAE by squaring the residuals before averaging.

It is useful for situations where larger errors are particularly undesirable.

These metrics collectively provide a comprehensive view of model performance. While R^2 offers a measure of how well the model explains the variance in the data, MAE and RMSE quantify the prediction errors. RMSE is more sensitive to outliers than MAE, making it particularly important in datasets with skewed distributions like the one used in this study.

3. Results and Discussion

3.1 Model Performance

The models were evaluated based on their ability to predict the corrosion rate of magnesium alloys using a variety of machine learning algorithms. The performance of each model was assessed using the **R^2 score**, which quantifies the proportion of variance in the target variable (corrosion rate) that is explained by the model. The R^2 score ranges from 0 to 100%, where a higher value indicates better model performance.

The results for each model are shown below table 1:

	R2 Score (%)	MAE	RMSE
LightGBM	59.939	0.255	0.591
Tuned Random Forest	47.806	0.218	0.675
Gradient Boosting	46.186	0.224	0.685
XGBoost	42.798	0.190	0.706
K-Nearest Neighbors	8.907	0.242	0.891
Support Vector Regression	2.796	0.318	0.921
Neural Networks	-12.871	0.418	0.992

As shown in the table 1 above, **LightGBM** outperformed all other models with an R^2 score of **59.94%**, indicating the highest accuracy in predicting the corrosion behaviour of magnesium alloys.

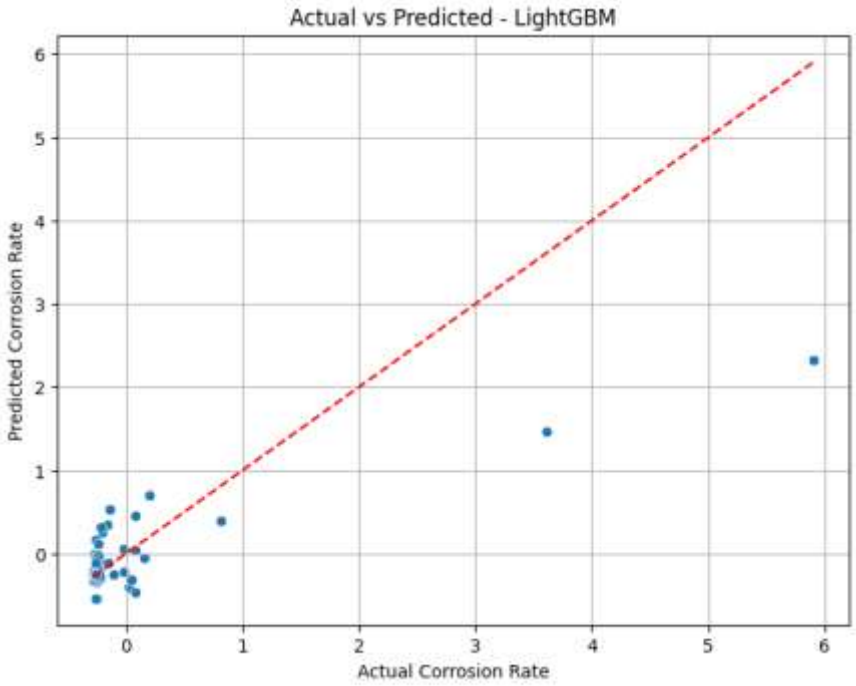

Figure 1. Actual vs Predicted corrosion rates using the LightGBM model. The red dashed line represents the ideal prediction line (y = x).

Figure 1 illustrates the relationship between the actual corrosion rates obtained from experimental studies and the predicted corrosion rates generated by the LightGBM model. Each point on the scatter plot represents a single magnesium alloy sample, with the x-axis showing the actual corrosion rate and the y-axis representing the corresponding predicted value. The red dashed line, drawn at a 45-degree angle, serves as the ideal reference line (y = x), indicating perfect prediction accuracy.

The majority of the data points lie close to this ideal line, particularly those representing lower corrosion rates, which form the bulk of the dataset. This close clustering suggests that the LightGBM model performs well in learning and predicting the general trends and behaviours associated with low corrosion rates. The proximity of these points to the diagonal indicates a minimal error between the model's prediction and the experimental values, signifying a high level of predictive precision for the most frequent cases.

However, several points are visibly dispersed further away from the line, especially those at higher corrosion rate values. These outliers indicate instances where the model's predictions deviate significantly from the actual outcomes. Such deviations are likely attributed to the limited number of high-corrosion-rate samples in the training data, resulting in insufficient learning about these extreme cases. This imbalance in data distribution hampers the model’s ability to generalize effectively for these rarer occurrences.

Despite the presence of outliers, the overall pattern of the scatter plot supports the conclusion that LightGBM is capable of accurately predicting corrosion rates for the majority of samples. The model captures complex interactions between alloy composition and environmental factors, and performs particularly well within the typical operating range relevant to biomedical applications.

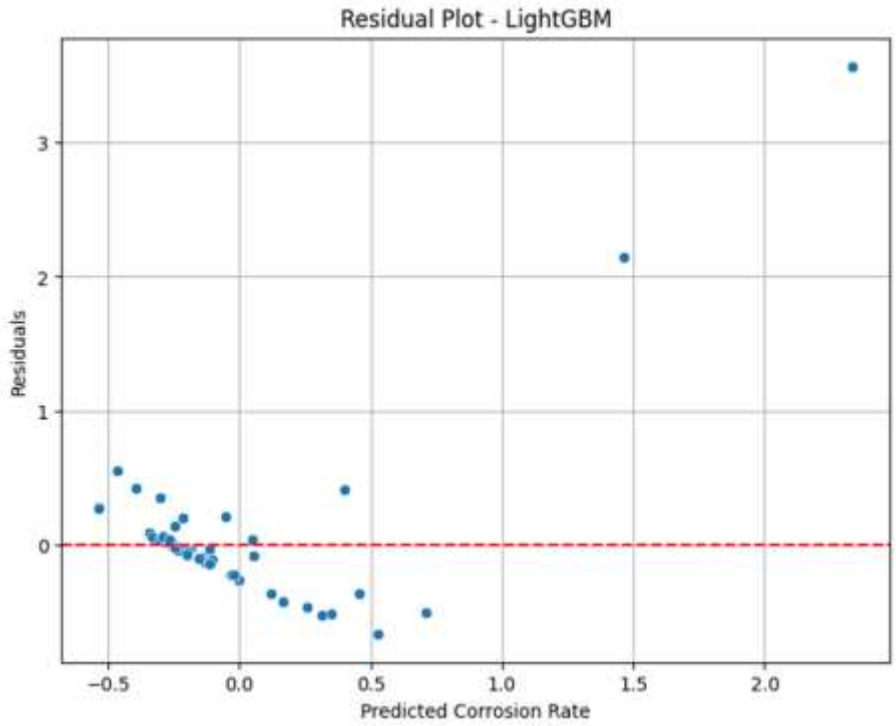

Figure 2. Residual plot of LightGBM predictions. Residuals are mostly centred near zero, indicating good model accuracy for most samples.

Figure 2 displays the residual plot corresponding to the LightGBM predictions. Residuals are defined as the difference between the actual corrosion rate and the predicted corrosion rate for each data point. An ideal regression model should produce residuals that are randomly scattered around zero without exhibiting any discernible pattern, which would indicate that the model's predictions are unbiased across the entire range.

In this plot, the residuals are plotted against the predicted corrosion rates. A large concentration of residuals appears close to the zero line, particularly in the range of low predicted corrosion rates, suggesting strong model performance in this domain. The clustering of residuals in this region indicates low prediction error and confirms that the model generalizes well to the dominant corrosion range in the dataset.

However, the plot also shows increasing dispersion in residual values as the predicted corrosion rate rises. A few residuals significantly deviate from zero, highlighting underprediction or overprediction in a small number of cases. These outliers likely correspond to rare samples with unusually high corrosion rates, as previously discussed in Figure 1. The presence of these larger residuals indicates that while the model performs well on common cases, it struggles with outliers and more complex or underrepresented conditions.

Furthermore, the residual plot does not show any systematic curve or funnel shape, which would have indicated heteroscedasticity (i.e., non-constant variance in the prediction error). This observation supports the assumption that the LightGBM model maintains consistent error variance, making it suitable for practical prediction in materials engineering contexts. Overall, this figure validates the model’s effectiveness, while also pointing to areas where model performance could be further refined through additional data enrichment or advanced regularization techniques.

3.2 Comparison of Model Performance:

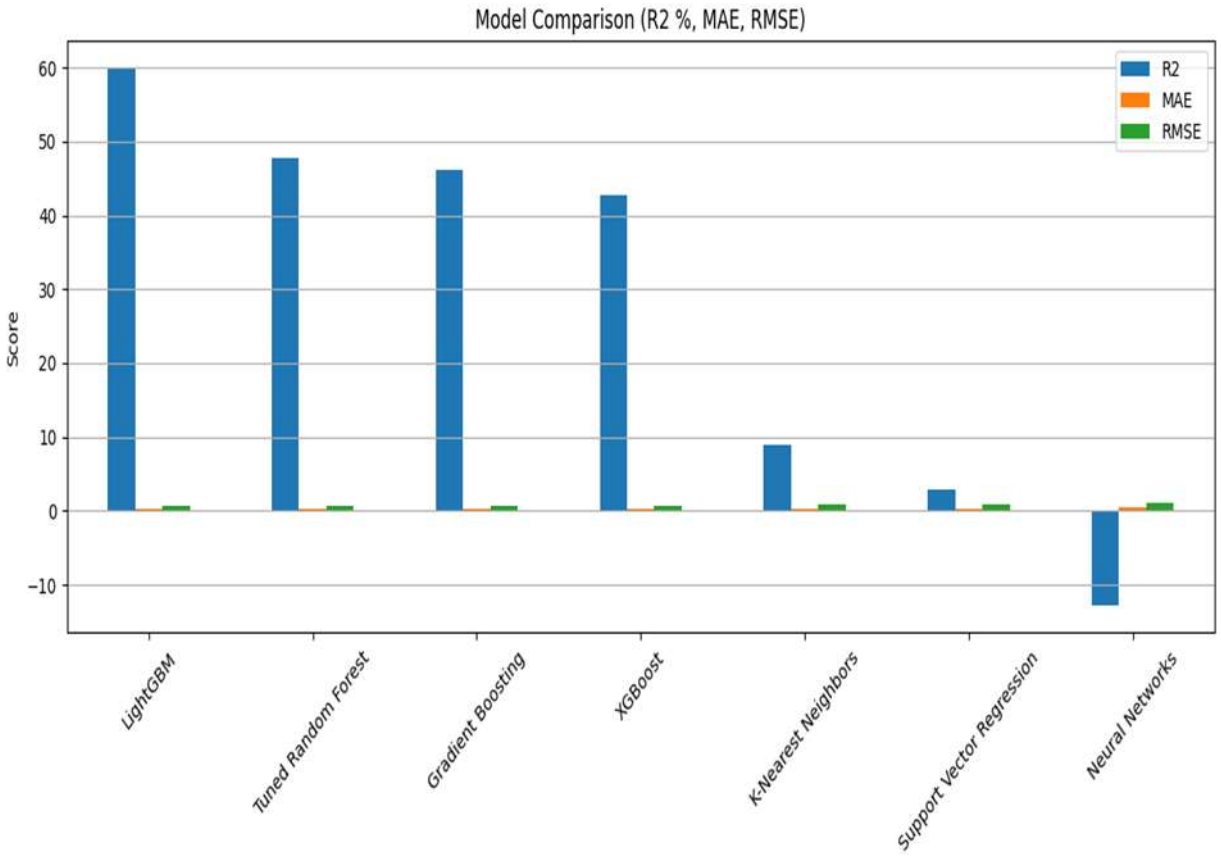

Figure 3:

The R^2 scores are visualized in the following graph to better compare model performances:

The graph clearly shows that **LightGBM** outperformed other models, followed by Random Forest and Gradient Boosting. Models such as SVR, KNN, and Neural Networks performed poorly, possibly due to sensitivity to data noise or insufficient complexity to capture underlying patterns.

3.3 Explanation of LightGBM's Superior Performance

LightGBM (Light Gradient Boosting Machine) is a gradient boosting framework that is optimized for performance, scalability, and accuracy. It is known for its efficiency in handling large datasets and its ability to capture complex patterns through boosting. Several factors contribute to LightGBM's strong performance in this study:

1. **Handling of Large and Complex Data**: LightGBM is particularly suited for handling large datasets with a large number of features. The high dimensionality in the dataset, including alloy composition, processing methods, and experimental conditions, is effectively managed by LightGBM's architecture.
2. **Feature Interaction Capture**: The algorithm's gradient boosting approach allows it to capture complex interactions between features, which may not be fully captured by simpler models like Random Forest or K-Nearest Neighbours.
3. **Regularization**: LightGBM includes regularization techniques, such as leaf-wise tree growth, which help prevent overfitting and improve the model's generalization ability, particularly on unseen data.
4. **Efficient Training**: Light GBM's implementation allows for faster training times, which makes it well-suited for iterative feature selection and hyperparameter tuning, leading to more optimized model performance.

3.4 Interpretation of Results

The R^2 scores across models suggest that machine learning can reliably predict corrosion rates based on alloy composition, processing techniques, and environmental factors. LightGBM's strong performance confirms the utility of boosting algorithms in capturing non-linear relationships in materials data [26][28].

Traditional models such as KNN and SVR underperformed, which aligns with prior findings that these models struggle when faced with noisy, multi-dimensional datasets typical in materials science [29].

The successful use of machine learning—particularly LightGBM—demonstrates a significant step forward in alloy screening for biomedical applications. It enables faster, data-driven decision-making compared to traditional trial-and-error methods, which are both time-consuming and expensive [27][30].

A correlation heatmap was generated to explore the relationships between various elemental compositions and the corrosion rate (CR) of magnesium alloys used in bone implants (Figure 4). The heatmap visualizes the Pearson correlation coefficients, where:

- Red shades represent strong positive correlations (values close to +1), meaning as one feature increases, the other also tends to increase.
- Blue shades represent strong negative correlations (values close to -1), meaning as one feature increases, the other tends to decrease.
- White or light colours indicate weak or no correlation (values around 0).

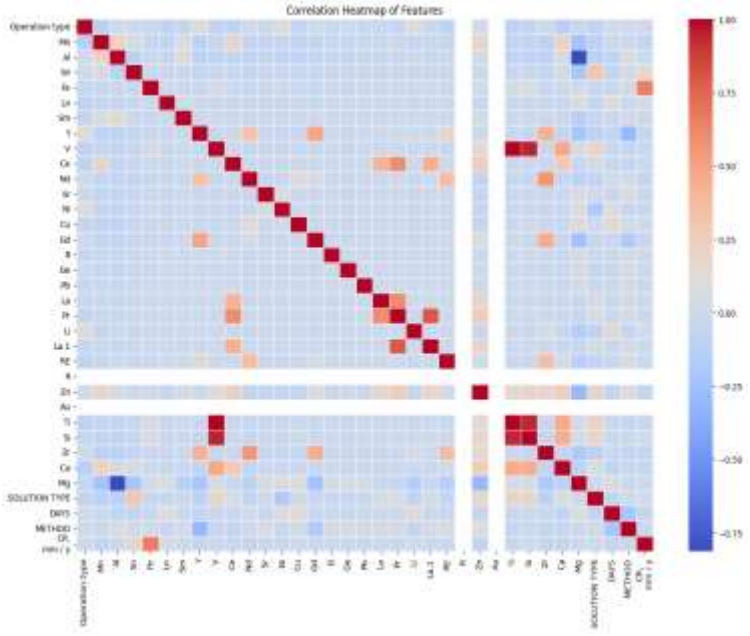

Figure 4: Correlation heatmap between elemental composition and corrosion rate.

Top 5 features most correlated with CR, mm / y:

	CR, mm/y
Fe	0.660
Sn	0.143
Mn	0.064
Ca	0.056
Nd	0.054

The strongest positive correlation with corrosion rate was observed for **Fe (Iron)**, with a correlation coefficient of **0.660**, indicating that a higher iron content tends to significantly increase the corrosion rate.

Boxplots of Top Correlated Features with Corrosion Rate

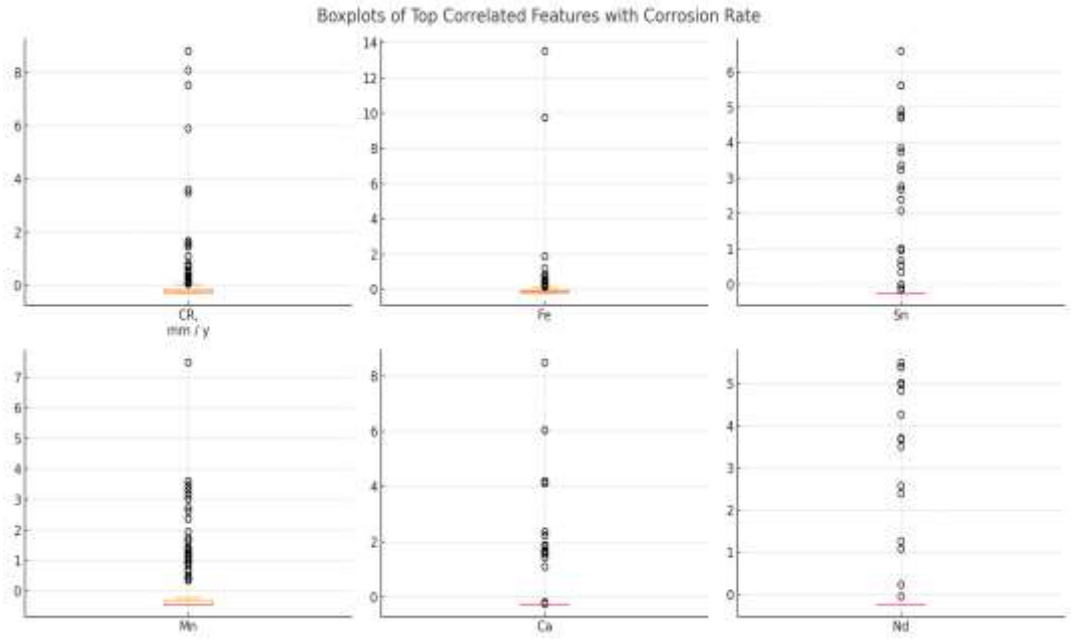

Figure 5: Boxplots of Top Correlated Features with Corrosion Rate

- The CR plot shows most samples corrode slowly, but a few extreme points reach over 200 mm/y.
- Fe has the strongest link to corrosion: higher Fe values align with higher CR.
- Sn also shows higher corrosion at its upper values, though less clearly than Fe.
- Mn, Ca, and Nd mostly stay at low levels; their few high-value points don't consistently raise CR.

4. Conclusion

This study presents a machine learning-based approach to predict the corrosion behaviour of magnesium alloys used in bone implants. The research integrates numerical alloy composition data, processing parameters, and experimental conditions to develop predictive models using multiple ML algorithms. Among the models evaluated, LightGBM achieved the highest prediction accuracy with an R^2 score, demonstrating its superior ability to handle complex, high-dimensional data.

The results confirm that machine learning, when combined with proper preprocessing, feature selection, and tuning, can effectively capture non-linear relationships between material features and corrosion performance. This offers a reliable, data-driven alternative to traditional trial-and-error methods in material selection.

By reducing the dependency on extensive experimental testing, the proposed ML framework enables faster and more cost-effective screening of biodegradable magnesium alloys. Such advancements can significantly accelerate the development of optimized bioresorbable implants, contributing to better patient outcomes and improved implant design in biomedical applications.

Future work may include expanding the dataset with additional features such as microstructural parameters, real-time in vivo data, and integrating deep learning techniques for enhanced prediction accuracy.

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