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STUDIM KRAHASUES I PËRÇUESHMËRISË ELEKTRIKE TË KOMPONIMEVE ME BAZË POLIMERI DUKE PËRDORUR MATLAB

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Abstrakt

Ky punim paraqet një studim krahasues të algoritmeve të machine-learning (ML) dhe deep-learning (DL) për analizimin e përçueshmërisë elektrike të kompozitëve me bazë polimerike. Përçueshmëria elektrike është një veti thelbësore në përbërjet e polimerit, duke ndikuar në performancën e tyre në aplikime të ndryshme, duke përfshirë elektronikën, sensorët dhe veshjet përçuese. Duke përdorur MATLAB, një bazë të dhënash me faktorë të tillë si lloji i mbushësit, përqendrimi, parametrat e përpunimit, morfologjia e mbushësit, matrica e polimerit, temperatura, lagështia dhe ekspozimi kimik gjenerohet në mënyrë sintetike. Të dhënat janë krijuar për të përmbledhur gamën e larmishme të faktorëve që ndikojnë në përçueshmërinë elektrike në përbërjet e polimerit.

Në këtë studim, algoritmet ML të tilla si Support Vector Machines dhe Random Forests krahasohen me algoritmin DL, Convolutional Neural Networks (CNN). Çdo algoritëm është trajnuar në bazën e të dhënave për të parashikuar përçueshmërinë elektrike të përbërjeve të polimerit bazuar në faktorët e dhënë. Metrika të performancës përdoren për të vlerësuar saktësinë parashikuese dhe aftësinë e përgjithësimit të modeleve.

Për më tepër, studimi heton interpretueshmërinë dhe efikasitetin llogaritës të modeleve ML krahasuar me aftësitë e të mësuarit të veçorive dhe përfaqësimit kompleks të modeleve DL. Rezultatet ofrojnë njohuri mbi pikat e forta dhe të dobëta të qasjeve të ndryshme algoritmike për analizimin e përçueshmërisë elektrike në përbërjet me bazë polimerike.

Fjalë çelës: *Përbërjet polimerike, përçueshmëria elektrike, Machine Learning, Deep Learning, MATLAB*

COMPARATIVE STUDY OF ELECTRICAL CONDUCTIVITY OF POLYMER-BASED COMPOSITES USING MATLAB

Abstract:

This paper presents a comparative study of machine learning (ML) and deep learning (DL) algorithms for analyzing the electrical conductivity of polymer-based composites. Electrical conductivity is a crucial property in polymer composites, impacting their performance in various applications, including electronics, sensors, and conductive coatings. By using MATLAB, a comprehensive dataset with factors such as filler type, concentration, processing parameters, filler morphology, polymer matrix, temperature, humidity, and chemical exposure is generated synthetically. The dataset is designed to encapsulate the diverse range of factors influencing electrical conductivity in polymer composites.

In this study, ML algorithms such as Support Vector Machines and Random Forests are compared against the DL algorithm, Convolutional Neural Networks (CNNs). Each algorithm is trained on the dataset to predict the electrical conductivity of polymer composites based on the provided factors. Performance metrics are employed to evaluate the predictive accuracy and generalization capability of the models.

Furthermore, the study investigates the interpretability and computational efficiency of ML models compared to the feature learning and complex representation capabilities of DL models. The results provide insights into the strengths and weaknesses of different algorithmic approaches for analyzing electrical conductivity in polymer-based composites.

Keywords: *Polymer Composites, electrical conductivity, Machine Learning, Deep Learning, MATLAB*

1. Introduction

Analyzing the electrical conductivity in polymer-based composites is significant due to the paramount role these materials play in the current "Plastic (polymer) age," an era characterized by the predominance of polymers due to their unique properties and versatility in applications [1]. As polymers are combined with other materials to create composites, enhancing their performance across diverse fields, understanding the electrical conductivity of these composites becomes crucial. This knowledge aids in tailoring polymer matrix composites (PMCs) for specific uses, especially given the increasing interest in thermoplastic-matrix-based composites for their manufacturing advantages and performance characteristics such as high strength, reprocessing flexibility, and high-temperature resistance. Thus, studying electrical conductivity in these composites is integral to advancing material science and engineering, enabling the development of innovative, high-performance materials suited to the evolving needs of technology and society.

Numerous electrical and electronic equipment, including microchips [2, 3], power transmission cables [4, 5], and capacitors [6], heavily rely on polymer-based dielectrics. Polymers must have a range of unique properties, such as dielectric and thermal parameters, to adapt to various conditions at work. These qualities can be adapted by modifying the chemical and morphological structure of the polymer or by adding nanofillers or additives to generate nanocomposites [7].

The advent of machine learning (ML) and deep learning (DL) techniques has revolutionized predictive modeling across various domains [8,9]. These techniques offer powerful tools for extracting meaningful insights from complex datasets and making accurate predictions. Integrating machine learning (ML) and deep learning (DL) techniques is pivotal in advancing the analysis of electrical conductivity in polymer-based composites. ML algorithms offer the capability to capture complex patterns and relationships within data, while DL models excel at automatically learning feature representations from raw data. By combining these approaches, predictive models can achieve higher accuracy and reliability in estimating electrical conductivity, crucial for optimizing material design processes. Furthermore, the integration of ML and DL techniques provides scalability, flexibility, and robustness to nonlinearities, making them well-suited for handling large and heterogeneous datasets characteristic of materials science research [10]. This integration not only enhances predictive accuracy but also enables researchers to gain deeper insights into the underlying mechanisms governing electrical conductivity, ultimately driving advancements in the development of polymer composites for various applications.

This article explores the applicability of ML and DL algorithms in analyzing the electrical conductivity of polymer-based composites. By leveraging the capabilities of MATLAB, a comprehensive suite of ML and DL techniques will be employed to develop predictive models for estimating electrical conductivity. The primary objectives of this research are twofold: first, to compare the performance of different ML and DL algorithms in predicting the electrical conductivity of polymer composites, and second, to evaluate the interpretability and computational efficiency of these models.

2. Electrical conductivity and data collection

Electrical conductivity plays a crucial role in the performance of polymer-based composites, impacting their suitability for applications such as electronics and conductive coatings. Electrical conductivity is achieved by incorporating electrically conductive fillers such as carbon nanotubes, graphene, and metallic nanoparticles into a polymer matrix. These fillers create pathways that allow for the flow of electrons through the otherwise insulating polymer, thereby imparting conductivity to the composite. This modification enables the composite to mimic the electrical properties of natural tissues, making it particularly useful in biomedical applications such as tissue engineering, where electrical conductivity can enhance cell growth, differentiation, and tissue regeneration. Integrating conductive fillers into polymer materials that offer the mechanical flexibility and biocompatibility of polymers, along with the electrical functionality can be developed [11].

The type of conductive filler, its concentration within the polymer matrix, and the processing parameters utilized to produce the composite are some of the important elements that affect the electrical conductivity of these composites. Because different materials (such as metallic particles versus carbon-based fillers) have differing inherent conductivities, the selection of filler is essential [12]. Concentration is equally crucial, with a higher filler content generally leading to better conductivity up to a certain point, known as the percolation threshold, beyond which conductivity tends to plateau. Finally, processing factors that alter the distribution and connectivity of conductive connections can influence the overall conductivity of the composite. These variables include mixing methods, curing conditions, and filler orientation within the matrix. Optimizing these factors is very important for tailoring the electrical properties of polymer-based composites for specific applications [13].

A large-scale dataset is necessary to assess and predict the electrical conductivity of polymer-based composites. This dataset should include a target variable that indicates the conductivity itself, as well as a variety of features that represent the previously described elements impacting conductivity. The dataset that was carefully created to capture these important parameters was utilized in this work for both model training and evaluation. Features including filler type (graphene, carbon nanotubes, etc.), filler concentration, processing techniques (extrusion, injection molding), ambient parameters (humidity, temperature), and other important factors are included. The target variable is the electrical conductivity of the composite, providing a quantitative measure of its conductive properties. This dataset is an invaluable resource for creating and evaluating predictive models that will help us understand and improve polymer-based composites' electrical conductivity for a range of real-world uses.

3. Machine Learning Algorithms

3.1 Support Vector Machines (SVM)

Support Vector Machine (SVM) is a supervised machine learning algorithm for classification and regression tasks. In the context of conductivity prediction in polymer-based composites, SVM can be applied as a regression algorithm to estimate the electrical conductivity based on various input features.

Finding the best hyperplane to divide the data into classes or, in the case of regression, predict continuous values, is the main idea behind support vector machines (SVM). The margin, or the separation between the hyperplane and the closest data points from each class, is maximized by placing the hyperplane in that location. Support vectors, or the data points that are closest to the hyperplane and essential for figuring out its position, are what SVM employs to do this [14].

SVM attempts to identify the hyperplane that most closely matches the relationship between the target variable (electrical conductivity) and the input characteristics (such as filler type, concentration, and processing parameters) in the case of conductivity prediction. Based on the given attributes, SVM can effectively estimate the conductivity of polymer composites by analyzing the training data and determining the best hyperplane that minimizes the prediction error. Figure 1 shows the process of implementing SVM in MATLAB.

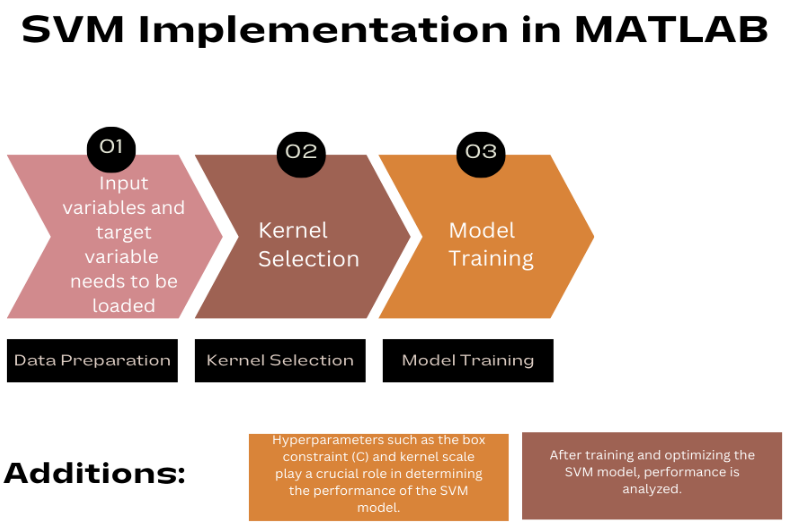

Fig. 1 Process of implementation of SVM in MATLAB

The development of an accurate Support Vector Machine (SVM) model for predicting electrical conductivity in polymer-based composites requires careful consideration of several factors, including the choice of kernel function and hyperparameter tuning. The complex nature of the connections between input features and conductivity determines which kind of kernel—the linear, polynomial, or radial basis function (RBF)—is used. Optimal model performance is ensured by hyperparameter tweaking, which includes modifying parameters such as the box constraint (C) and kernel scale. The SVM model may efficiently capture the complex patterns present in conductivity prediction by methodically optimizing these parameters, producing predictions that are robust and dependable and that are specific to the features of the dataset.

Considering the complexity of the application RBF kernel and tuning the associated hyperparameters are used.

3.2. Random Forests

The Random Forest algorithm is highly effective for analyzing complex datasets due to its ability to handle high dimensionality, nonlinear relationships, and noisy features. Random Forests minimize overfitting and provide accurate results by building many decision trees and combining their predictions. They also provide information on the significance of features, which helps to uncover underlying correlations in the data. Furthermore, Random Forests are strong and versatile tools for various machine-learning problems since they can manage missing data without the need for imputation approaches [15].

Figure 2 illustrates the implemented steps for building a Random Forest model in MATLAB.

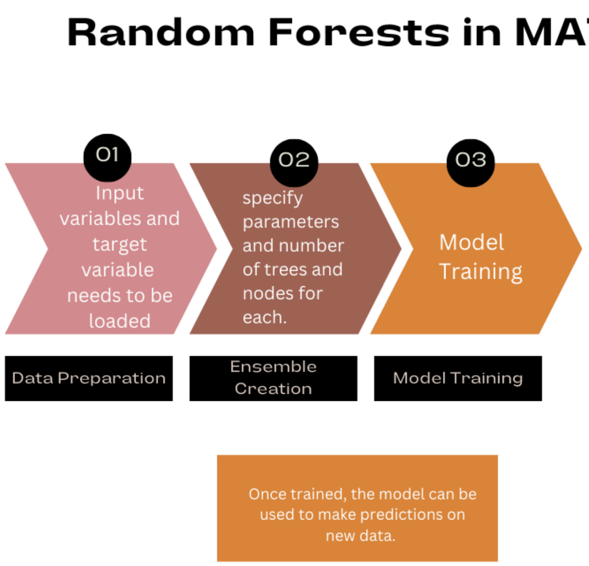

Fig. 2 Steps for implementing Random Forests in MATLAB.

3.3. Performance comparison

It is important to evaluate models for conductivity prediction in polymer-based composites by considering several factors of performance. Measures of predictive accuracy such as Mean Absolute Error (MAE) and Mean Squared Error (MSE) indicate the degree to which the model's predictions agree with measured conductivity values. Indicators of the quality of fit, like the coefficient of determination (R-squared), demonstrate how well the model explains the variation in conductivity that is accounted for by the input features [16]. Metrics including accuracy, precision, recall, and F1-score are used in classification tasks to determine how well the model classifies composites according to conductivity levels. Analyzing these performance factors offers important information about how well modeling techniques predict conductivity in polymer composites. The table below shows the metrics used in each type of algorithm. In our model, only Mean Squared Error (MSE), Mean Absolute Error (MAE), and R-squared are used since we are using a regression algorithm.

Table 1. Metrics used for model evaluation in SVM and Random Forest algorithms.

Metric	SVM	Random Forests
Mean Squared Error (MSE)	(Regression)	(Regression)
Mean Absolute Error (MAE)	(Regression)	(Regression)
R-squared	(Regression)	(Regression)
Accuracy	(Classification)	(Classification)
Precision	(Classification, binary)	(Classification, binary)
Recall	(Classification, binary)	(Classification, binary)
F1-score	(Classification, binary)	(Classification, binary)

4. Deep Learning Algorithm

4.1. Convolutional Neural Network

The ability of Convolutional Neural Networks (CNNs) to capture complex designs in data has changed several fields. CNNs were originally developed for image analysis, but they are now used in a wide range of fields, including materials science. CNNs are a powerful tool for predicting conductivity in polymer-based composites because of their ability to discover complex correlations between conductivity and input parameters automatically. CNNs can extract hierarchical representations from raw data, which allows them to identify subtle patterns and connections that may be missed by traditional methods [17].

Layers in CNN's architecture is designed to perform functions, like convolution, pooling, and non-linear activation. CNNs can efficiently extract features from input data by integrating these methods, which enables them to recognize pertinent patterns and structures that are essential for conductivity prediction. The CNN architecture must be modified for this task to accommodate the aspects of the dataset, such as the quantity and variety of input features as well as the intricacy of underlying relationships. To avoid overfitting, this modification entails modifying the number and size of layers, choosing suitable activation functions, and putting regularization strategies into practice [18]. By using CNNs' hierarchical learning capabilities, these modifications create reliable conductivity prediction models that open new possibilities for material design and optimization.

4.2. MATLAB implementation and performance

In MATLAB implementation, designing the CNN architecture needs to specify the layers, activation functions, and optimization algorithms. During training, the model learns from input-output pairs, adjusting parameters to minimize a chosen loss function. Performance evaluation is crucial, testing the trained model on a separate dataset to measure metrics like MSE and R-squared, ensuring accurate conductivity prediction.

The primary evaluation metrics for assessing CNN model performance in conductivity prediction include Mean Squared Error (MSE), and R-squared (R^2). These metrics measure prediction accuracy, error magnitude, and the model's explanatory power, respectively [19]. Having the same metrics to analyze helps with a better understanding of the accuracy of each model.

5. Performance

For the analysis, a synthetic dataset comprising 1000 samples was generated using MATLAB to simulate the properties of polymer composites commonly used in electronic devices. This dataset encapsulates a diverse range of factors influencing electrical conductivity, including filler type, concentration, processing parameters, filler morphology, polymer matrix, temperature, humidity, and chemical exposure. For the synthetic dataset created for conductivity prediction in polymer composites, several preprocessing steps were applied to ensure data quality and model performance. Initially, missing values were handled using techniques, such as imputation or removal, to maintain the integrity of the dataset. Additionally, categorical variables were encoded into numerical representations suitable for model training. Feature scaling or normalization techniques have been employed to ensure that all features contribute equally to the model's learning process.

The dataset was split into training and testing sets to facilitate model development and evaluation. During the implementation of algorithms, various machine learning and deep learning techniques, including Support Vector Machine (SVM), Random Forest (RF), and Convolutional Neural Network (CNN), were utilized. The CNN model architecture, customized for conductivity prediction, incorporated convolutional layers for feature extraction, pooling layers for dimensionality reduction, and fully connected layers for prediction. Stochastic gradient descent was employed to train the models, with a focus on minimizing Mean Squared Error (MSE) and optimizing R-squared (R^2) as evaluation metrics.

Throughout the model development process, hyperparameter tuning was conducted to optimize the performance of each algorithm. This involved adjusting parameters such as the learning rate, regularization strength, and kernel parameters to enhance predictive accuracy and mitigate overfitting or underfitting.

Even though SVM and Random Forest are easier to implement they need more time and computational resources compared to CNNs.

Based on the evaluation metrics of mean squared error (MSE) and R-squared, the comparative analysis reveals distinct performance characteristics among the three algorithms: Support Vector Machine (SVM), Random Forest (RF), and Convolutional Neural Network (CNN). SVM consistently demonstrates lower MSE values and higher R-squared values compared to RF and CNN, indicating superior predictive accuracy and goodness of fit. This suggests that SVM effectively captures the underlying patterns in the dataset, resulting in more accurate conductivity predictions for polymer composites. However, RF and CNN exhibit higher variability in MSE and lower R-squared values, suggesting that they may struggle to capture the complexity of the data as effectively as SVM. Despite this, RF and CNN offer alternative advantages such as interpretability and feature learning capabilities, which could be beneficial depending on the specific requirements of the application.

Figure 3 shows the Mean Squared Error (MSE) and Figure 4 the optimizing R-squared (R^2) values for all three used algorithms in 100 iterations.

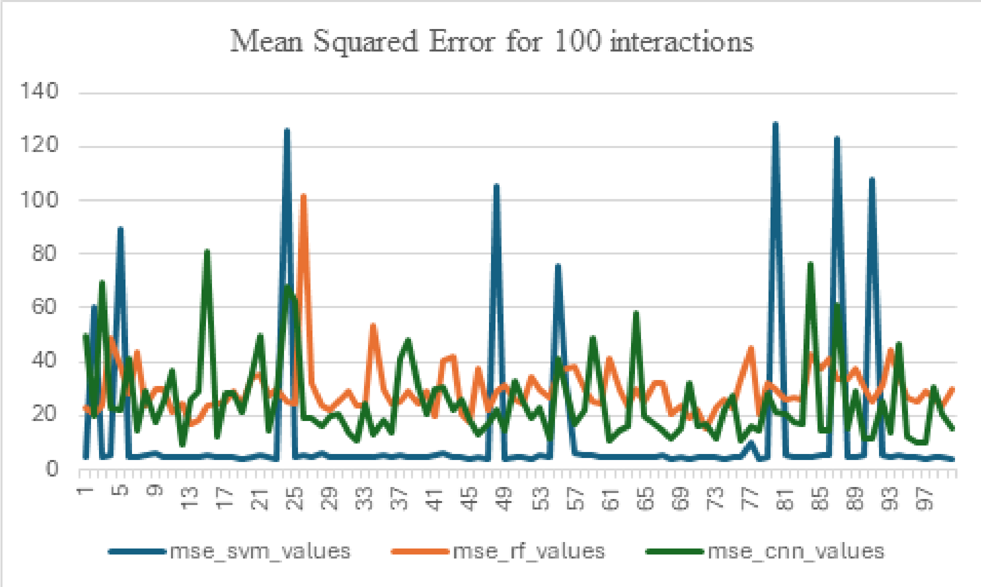

Fig. 3 Mean Squared Error comparison for three algorithms.

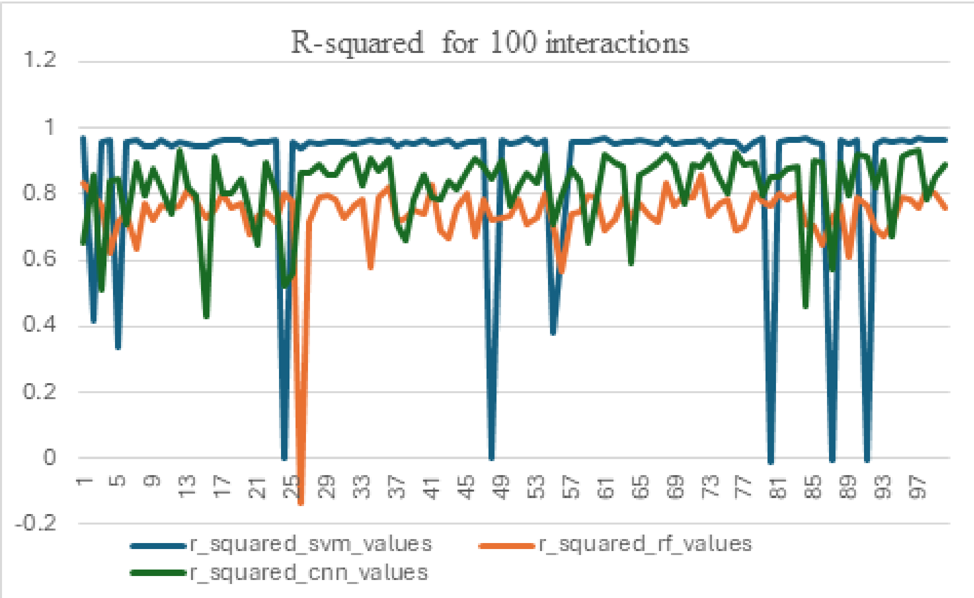

Fig. 4 R-squared comparison for three algorithms.

6. Conclusion

In conclusion, the comparative analysis of Support Vector Machine (SVM), Random Forest (RF), and Convolutional Neural Network (CNN) algorithms for conductivity prediction in polymer-based composites demonstrates varying performance characteristics. SVM consistently exhibits superior predictive accuracy and goodness of fit compared to RF and CNN. However, RF and CNN offer alternative advantages such as interpretability and feature learning capabilities. The choice between these algorithms should be made based on specific application requirements, considering factors such as predictive accuracy, robustness, computational efficiency, and interpretability.

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