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Accurate Prediction of Polymer Specific Heat Capacity Using Advanced Machine Learning Techniques

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1. ABSTRACT

This study focuses on predicting the specific heat of polymers using experimental data and machine learning algorithms. A comprehensive dataset comprising physical and chemical properties of polymers was utilized as input for various models, including linear regression, Ridge, Lasso, ElasticNet, K-nearest neighbors, artificial neural networks, and decision trees. The performance of these models was evaluated using mean squared error (MSE) and R-squared (R^2) metrics. The results indicate that the Lasso and ElasticNet models provide the best balance between accuracy and generalization to new data. Specifically, the Lasso model achieved an MSE of 728.77 and an R^2 of 0.95, while the ElasticNet model recorded an MSE of 604.34 and an R^2 of 0.95. This study emphasizes that employing regularization techniques and ensemble models can significantly enhance the accuracy and stability of predictions for the thermal properties of polymers, leading to substantial savings in both time and costs associated with experimental testing.

Keywords: Thermal Property, Machine Learning, Intelligent Algorithms, Specific Heat, Polymers.

2. INTRODUCTION

Thermal Polymers are widely recognized as engineering materials with applications in automotive, packaging, electronics, and medical industries due to their lightweight, design flexibility, and thermal and chemical stability. Among the various properties of polymers, specific heat capacity holds significant importance due to its direct impact on processes such as heat transfer, thermal shaping, and thermal control. While experimental measurement of this property using advanced devices like differential scanning calorimetry (DSC) is accurate, it is often time-consuming, costly, and limited to specific laboratory conditions. Thus, the emergence of data-driven methods, particularly machine learning (ML), presents an effective, rapid, and economical approach for predicting the specific heat capacity of polymers [1-2].

3. MATERIALS AND METHODS

3.1. Data Used in the Study

This research utilized a dataset comprising structural, physical, and chemical characteristics of various polymer samples. The dataset included numerous samples, each with multiple recorded molecular feature values, sourced from literature [3]. Specific heat capacity was treated as the target variable, while the input variables included structural properties and

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descriptors that directly or indirectly influence the thermal characteristics of polymers. A total of 188 input features were recorded for each sample, which were then normalized and preprocessed before being divided into 80% for training and 20% for testing.

3.2. Modeling Methods

The modeling process was structured and systematic, involving the use of libraries such as NumPy, Pandas, Matplotlib, Seaborn, and Scikit-learn. After initial data examination and cleaning, various machine learning algorithms were employed, including linear regression, regularized regression (Ridge, Lasso, ElasticNet), K-nearest neighbors (KNN), artificial neural networks (ANN), and decision trees. Model performance was evaluated using metrics such as the coefficient of determination (R^2) and mean squared error (MSE)

4. RESULTS AND DISCUSSION

Multiple machine learning models were assessed for their ability to predict the specific heat capacity of polymers. The results demonstrated that while classical linear regression exhibited high R^2 values (0.99) and low MSE during training, it performed poorly on test data due to severe overfitting. In contrast, regularized models (Ridge, Lasso, and ElasticNet) significantly mitigated overfitting and showed better generalization to test data, with Lasso and ElasticNet achieving the best balance between accuracy and generalizability.

The following Table 1 summarizes the performance metrics of different models:

Table 1. Performance metrics of different models

Model	R^2 - Testing	R^2 - Training	MSE- Testing	MSE - Training
Linear Regression	0.10	0.99	1841989545	0.38
Ridge Regression	0.89	0.99	11.15	41.42
Lasso Regression	0.95	0.99	77.77	88.08
Elastic Net	0.95	0.98	34.34	167.58
K-Nearest Neighbors (KNN)	0.82	0.78	2500.37	2247.68
Artificial Neural Network	0.94	0.99	751.06	2.05
Decision Tree	0.82	0.96	2548.29	401.44
Random Forest	0.90	0.98	1402.85	187.43

Artificial neural networks (ANN) also showed promising results, with the Scikit-learn implementation yielding an R^2 of 0.94 on test data, indicating high accuracy and generalizability. However, the Keras implementation demonstrated signs of overfitting. Decision tree models showed limited generalization, while Random Forest models improved performance through ensemble techniques

5. CONCLUSION

The study concluded that machine learning models, particularly Lasso and ElasticNet, provided effective tools for predicting the specific heat capacity of polymers, offering a reliable alternative to costly experimental methods. Future research should focus on optimizing ANN structures and hyperparameters, employing advanced regularization methods, and expanding datasets to enhance predictive accuracy. Overall, this research highlights the potential of machine learning in polymer engineering, paving the way for smarter material selection and design processes.

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