International Journal of
INTELLIGENT SYSTEMS AND APPLICATIONS IN ENGINEERING
ISSN:2147-6799 www.ijisae.org Original Research Paper

Advancing Polymer Property Prediction through Machine Learning: A Focus on Melting Temperature and Molecular Parameter-based ANN Modeling

Ms. S. Bhuvaneswari[1], Dr.A.Abirami[2], Ms. D. Kavitha[3], Harishma S[4], Hardlin Sherin R[5], Devnanda Kurup[6], Kishore Kumar B[7], Rajkumar S[8], Sai Vikram Karna A[9]

Submitted: 29/01/2024 **Revised**: 07/03/2024 **Accepted**: 15/03/2024

Abstract: Polymeric materials play a pivotal role across numerous applications, driving innovation in various sectors. However, evaluating the properties of polymers traditionally involves costly and time-consuming experimental procedures. In this document, we explore the application of computational approaches, particularly machine learning (ML), in predicting crucial polymer properties, with a focus on the melting temperature (Tm). We introduce an Artificial Neural Network (ANN) model trained on molecular parameters to accurately predict Tm, demonstrating its effectiveness and affordability in comparison to conventional techniques. Additionally, we delve into the significance of polymer fingerprinting techniques, particularly Extended-Connectivity Fingerprints (ECFP), in encoding complex polymer structures for ML applications. Furthermore, we discuss feature engineering techniques such as Feature Selection and Feature Extraction, essential for refining input data and optimizing model performance. Finally, we detail the development of our ML model, including integration layers, optimization strategies, and hyperparameter tuning, emphasizing its potential for advancing polymer science and engineering. This comprehensive approach opens up new possibilities for material research and design while also advancing our understanding of polymer behavior.

Keywords: artificial neural network, fuzzy logic, polymer fingerprinting**,** simplified molecular input line entry system

1. Introduction

Polymeric materials hold immense significance across various domains, profoundly influencing human life through their diverse applications. The quest for improved performance metrics such as enhanced strength, reduced weight, and minimized environmental impact has fueled extensive exploration into novel polymers and the reevaluation of existing materials. However, traditional methods for evaluating candidate materials incur significant costs, prompting a shift towards computational approaches as a viable alternative. Understanding polymeric materials requires consideration of their hierarchical structure, spanning multiple length scales from molecular details to macroscopic dimensions. Molecular characteristics dictate structural stability, while chain interactions and domain formations at the mesoscale affect properties like elasticity and permeability. At a macroscale level, factors such as processing conditions and dimensions impact characteristics like optical transparency and tensile strength. Developing effective multiscale modeling approaches is essential for comprehensively understanding polymeric materials, although traditional methods may be limited in exploring a large number of materials due to extensive simulations and complex algorithms. Machine learning (ML) techniques have emerged as promising tools in predicting polymer properties, with successful applications in forecasting parameters like glass transition temperature (Tg) and tensile strength. Leveraging ML methods such as support vector regression and artificial neural networks (ANN) has proven effective in accurately predicting complex polymer properties. Shifting focus to predicting the melting temperature (Tm) of polymers through ANN introduces a transformative approach, addressing limitations of traditional experimental methods such as DSC and DMA. Our research employs ANN to predict Tm by exploring relationships between molecular parameters and polymer characteristics. ANNs, known for their pattern recognition capabilities, enhance prediction efficiency at a low cost, contributing to a deeper understanding of polymer behavior. The ANN architecture involves convolutional layers for feature extraction from encoded monomer structures, followed by flattening and fully connected layers for processing and prediction. Optimization strategies like customized loss functions and hyperparameter tuning enhance model robustness and efficiency. The developed ANN model offers a rapid, accurate, and cost-effective means of predicting Tm, aiding in polymer design and enhancing comprehension of complex molecular relationships. Its ability to generalize patterns and learn relationships makes it a valuable asset in polymer science and engineering, opening innovative avenues for material design and development.

Computer science and Engineering Easwari engineering college, Ramapuram,Chennai-89 bhuvaneswarisoman@gmail.com [1], abiavsbtech@gmail.com [2], dkavithavijay@gmail.com [3], harishma.055@gmail.com [4], hardlinsherin@gmail.com [5], devnandakurup01@gmail.com [6], kishorekumar.bcseb@gmail.com [7]], rajkumarsambath54@gmail.com [8], saivikramkarna08@gmail.com [9]
** Corresponding Author Email: bhuvaneswarisoman@gmail.com*

2. EXPERIMENTAL METHODS

2.1. Polymer Data Acquisition

The polymer dataset employed in this study was sourced from Khazana, a reputable repository renowned for its extensive collection of polymer data. This dataset comprises a diverse range of features essential for the comprehensive analysis and prediction of polymer properties. Notably, the dataset includes Atomization Energy (Eat), which quantifies the energy required to disassemble a polymer into its constituent atoms per atom. Additionally, Crystallization Tendency (Xc) is represented as a percentage, indicating the likelihood of polymer crystallization. Band Gap

Chain (Egc) and Band Gap Bulk (Egb) features denote the energy disparity between the conduction and valence bands in polymer chain and bulk states, respectively. Furthermore, Electron Affinity (Eea) and Ionization Energy (Ei) metrics quantify the energy necessary for adding or removing electrons from polymer molecules. Refractive Index DFT (nc) and Dielectric Constant DFT (eps) offer insights into the optical and electrical characteristics of polymers. This comprehensive feature set provides a solid foundation for in-depth analysis and modeling of polymer behavior, thereby facilitating advancements in material design, characterization, and optimization.

Ahead of delving into individual module explanations, the (Figure 1) elucidates the hierarchical arrangement and interdependencies of the system components, offering insights into the flow of data and processing steps.

Table 1. Polymer Properties

SMILES	Atomization Energy (Eat)	Crystallization Tendency (Xc)	Band Gap Chain (Egc)	Band Gap Bulk (Egb)	Electron Affinity (Eea)	Ionization energy (Ei)	Refractive index (nc)	Dielectric constant (eps)
[*]CO[*]	-5.32	97.7431466	6.6048	8.7732	0.9897	7.5826	1.6434	3.72
[*]CCO[*]	-5.21	70.6655082	5.5372	6.2206	0.3936	7.0344	1.6377	3.15
[*]CCCO[*]	-5.2	55.46	6.2459	7.4889	0.5672	6.904	1.6476	3.03
[*]CC([*])C	-5.14	44.47	6.5196	7.6997	0.4343	6.185	1.6081	2.61
[*]CCC(=O)O[*]	-5.73	45.0097846	7.0337	6.684	0.7562	7.7853	1.6631	3.39
Number of Samples	390	431	3379	560	457	369	381	381

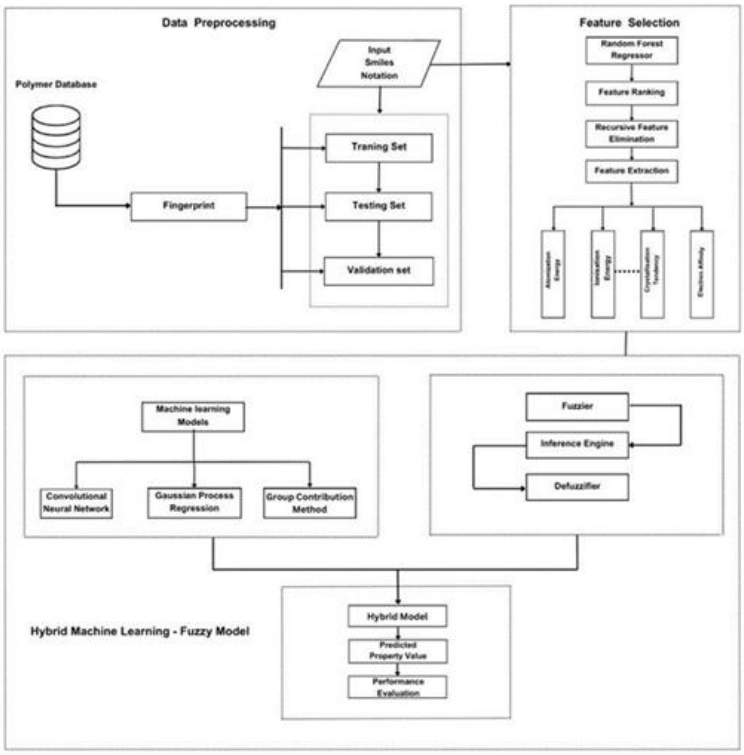

Figure 1. Architecture Diagram

2.2. Conversion of SMILES

The process of converting polymer names into Simplified Molecular Input Line Entry System (SMILES) notation involves several steps aimed at representing the chemical structure of polymers in a standardized format. In this study, an automated approach was employed for SMILES conversion to ensure efficiency and accuracy. Specifically, the polymer names were inputted into a specialized software tool designed for chemical structure representation. One such commonly used software is the RDKit library in Python, which provides a range of functions for handling chemical data, including SMILES conversion. The RDKit library utilizes algorithms and databases to interpret polymer names and generate corresponding SMILES strings. These strings encapsulate the structural information of polymers in a concise and machine-readable format, facilitating further analysis and modeling. By leveraging automated tools like RDKit, the SMILES conversion process ensures consistency and reliability in representing polymer structures for subsequent feature engineering and modeling tasks.

2.3. Extraction of Features

Feature engineering involves the systematic process of extracting or generating relevant features from the SMILES representations of polymers to facilitate subsequent analysis and modeling. In this study, feature engineering was conducted with a focus on

extracting informative features from the chemical structures encoded in SMILES notation. A specific technique employed for feature selection was Recursive Feature Elimination (RFE), a widely used method in machine learning for identifying the most relevant features. RFE systematically removes features from the dataset while training the model and evaluates the model's performance at each iteration. By iteratively selecting and removing features based on their importance, RFE identifies the subset of features that contribute most significantly to predicting polymer properties. Additionally, other feature extraction techniques, such as molecular fingerprinting methods like Extended-Connectivity Fingerprints (ECFP), were utilized to capture the structural characteristics of polymers. These techniques encode molecular structures into numerical representations, enabling the extraction of relevant features for modeling. Overall, feature engineering in this study aimed to enhance the predictive performance of the models by selecting and generating informative features from the SMILES representations of polymers.

2.4. Fuzzy Logic Integration

After performing feature engineering to extract relevant features from the polymer data, the next step involves integrating fuzzy logic techniques to handle uncertainty and imprecision in the input data. Fuzzy logic operates through several key steps to achieve this. Firstly, in the fuzzification step, numerical input parameters are transformed into fuzzy sets using appropriate membership functions. These membership functions assign degrees of membership to linguistic terms, capturing the uncertainty inherent in polymer properties. Mathematically, fuzzification can be represented as Equation (1) :

$$\text{Fuzzification: } x \rightarrow \mu(x) \qquad (1)$$

Following fuzzification, fuzzy inference rules are applied in the inference engine. These rules encode expert knowledge or data-driven relationships between input features and polymer properties. The inference process combines the fuzzified input data with the fuzzy rules to generate fuzzy output values representing polymer characteristics. The fuzzy inference is stated as Equation (2) :

$$\text{Fuzzy Inference: Output} = f(\text{Input}) \qquad (2)$$

Finally, in the defuzzification step, fuzzy output values are converted into crisp numerical predictions using defuzzification techniques. This process extracts a single, actionable prediction from the fuzzy output values, facilitating decision-making in polymer property prediction. One common defuzzification method is the centroid method, which computes the center of gravity of the fuzzy output membership functions. The formula for defuzzification using the centroid method is expressed in Equation (3) :

$$y = \sum i \mu i \sum i (\mu i \cdot \text{Value}i) \qquad (3)$$

By integrating fuzzy logic techniques after feature engineering, uncertainties and imprecisions in the input data are effectively managed, resulting in a more robust representation for subsequent modeling of polymer properties.

2.5. Prediction of Polymer Property using Artificial Neural Networks

Predicting the melting temperature (Tm) of polymers plays a vital role in material science and engineering, as it governs a wide range of properties and applications. Artificial Neural Networks (ANNs) have emerged as powerful tools for this task, offering a data-driven approach to unveil the complex relationships between a polymer's structure and its thermal behaviour.

2.5.1. Input Data Representation

In predicting the melting temperature (Tm) of polymers using artificial neural networks (ANNs), input data quality is paramount. Typically, binary images encoding polymer structure are utilized. Each pixel in these images corresponds to a location within the polymer chain, with 1 representing atom presence and 0 indicating empty space. Techniques like zero-padding standardize image dimensions, crucial for unbiased consideration of structural features.

2.5.2. Processing through Hidden Layers

Hidden layers play a crucial role in ANNs, enabling the extraction of intricate patterns from input data. Within these layers, neurons receive activations from the preceding layer as inputs. Each neuron conducts computations by calculating a weighted sum of these inputs, modulated by learned weights and a bias term. The integration of non-linear activation functions, such as Rectified Linear Unit (ReLU), introduces essential non-linearity, facilitating the extraction and transformation of features within the network.

2.5.3. Training and Optimization

ANN training involves exposing the network to a dataset of polymer structures and their measured Tm values. Stochastic Gradient Descent (SGD) optimizes the network by iteratively updating weights and biases to minimize a loss function, measuring the variance between predicted and actual Tm values. SGD updates weights and biases based on gradients of the loss function, iteratively improving the network's comprehension of data and prediction accuracy. Other optimization methods like Adam and RMSprop offer adaptive learning rates for faster convergence. Weight Update (SGD) can be calculated as:

$$w_{ij}^{(t+1)} = w_{ij}^{(t)} - \eta \frac{\partial L}{\partial w_{ij}^{(t)}} \qquad (4)$$

In Equation (4) $w_{ij}^{(t)}$ represents the weight between neuron *i* in layer l−1 and neuron *j* in layer *l* at iteration *t*, η is the learning rate, and $\frac{\partial L}{\partial w_{ij}}$ is the loss function's gradient in relation to weight.

2.5.4. Output Layer

The output layer generates the final Tm prediction based on processed information from the last hidden layer. It computes the activation of a neuron using a weighted sum of inputs, with a bias term. Here, y_pred is computed by Equation (5)

$$y_{pred} = \sum_{j=1}^{k} w_j^{(L)} . h_j^{(L)} + b^{(L)} \qquad (5)$$

Where $w_j^{(L)}$represents the weight of the connection between neuron j in the last hidden layer and the output neuron, $h_j^{(L)}$ denotes the activation of neuron j in the last hidden layer, $b^{(L)}$ is the bias term for the output neuron and k is the number of neurons in the final hidden layer. The output represents the predicted Tm of the polymer based on learned patterns and relationships captured by the neural network.

3. Results And Discussion

3.1. SMILES Output

The (table 2) presents the conversion of polymer names to Simplified Molecular Input Line Entry System (SMILES) notation, providing a concise representation of polymer structures. Each entry in the table corresponds to a polymer sample, facilitating efficient data handling and analysis for predictive modelling.

Table 2. Polymer Name and Corresponding SMILES Notation

Sl.No	*Polymer Name*	*SMILES*
1	1,4-cyclohexanedimethanol	OC(=O)CCCCCCCCC(=O)O
2	1,12-dodecanedioic acid	C(CCCC(=O)O)CCCC(=O)O
3	neopentyl glycol	CCC(CO)(CO)CO
4	2,2,4,4-tetramethyl-1,3-cyclobutanediol	CC(CO)CO
5	1,4-cyclohexanedicarboxylic acid	OCCCO
6	isophthalic acid	OCCCO
7	azelaic acid	O=C(O)c1cccc(C(=O)O)c1
8	isophthalic acid	CCC(CO)(CO)CO
9	1,4-cyclohexanedicarboxylic acid	OCCCCCCO
10	trimethylolpropane	OCCCO

3.2. Chi-Square Test for Feature Extraction

The chi-square test is used by the system to determine whether each feature value in the table is independent or connected before extracting the Zoning feature. A contingency table is used in the test to assess the data. Both hypothesis H0: variable 1 is independent of variable 2, and hypothesis H1: variable 1 is not independent of variable 2, are ways to represent the Chi test. The test supports the assumed hypothetical probability fit to the observed data. Testing for homogeneity and attribute independence is the primary goal of the chi-square . Let the Observed variable be the polymer feature. The chi-square test of the independence test statistic is $\chi 2$, and it is computed as

$$\chi^2 = \sum_{i=1}^{r}\sum_{j=1}^{c}\frac{(O_{ij}-E_{ij})^2}{E_{ij}},$$

where Eij is the observed frequency of the polymer features in the contingency table's ith row and jth column and Oij is the forecasted frequency of the polymer features in the contingency table's ith row and jth column.The $\chi 2$ test is employed to evaluate the relationship between independent and dependent variables, particularly in feature extraction methods for polymer property prediction. If the computed $\chi 2$ value exceeds the critical value derived from the $\chi 2$ table, the null hypothesis (H0) is rejected. In contrast, if it falls within the critical value, the null hypothesis is acknowledged. In a recent analysis, the computed $\chi 2$ value was 2.923, surpassing the critical value of 15.51 for a 95% confidence level. Consequently, the null hypothesis is accepted, indicating that the zoning method's feature vector values are not independent. This underscores the dependency of observed polymer feature values on melting temperature, validating the effectiveness of the feature extraction method in predicting polymer properties.

Table 3. Chi-Square Test for Goodness of Fit Results

Category	O_i	E_i	$(O_i - E_i)2/E_i$
1	97	93.9	0.10
2	70	68.3	0.04
3	55	56.3	0.03
4	44	45.2	0.03
5	45	46.9	0.07
6	9	11.1	0.39
7	7	8.1	0.14
8	8	6.7	0.25
9	7	5.3	0.54
10	6	5.5	0.04
11	4	4.8	0.13
12	3	3.5	0.07

13	3	2.9	0.03
14	2	2.3	0.03
15	4	2.4	1.06
	364		$\chi^2 = 2.923$

3.3. Performance Evaluation of Machine Learning Techniques for Predicting Polymer Properties

A thorough quantitative assessment of the model's prediction accuracy is provided by the performance evaluation metrics, which include mean absolute error (MAE), coefficient of determination (R-squared), and median relative error (MRE). These metrics serve as foundational benchmarks for evaluating the efficacy of the ANN model in capturing the complex relationship between polymer structure and melting temperature.

3.3.1. Mean Squared Error (MSE) and R-squared (R2) Values

(Table 6) represents comparison graphs to illustrate the predictive accuracy of different machine learning techniques, including ANN, in predicting polymer properties. These graphs depict the predicted Tm values versus the actual Tm values for each model, allowing for a direct comparison of their performance. From the results, it is evident that the ANN model outperforms other machine learning techniques in terms of predictive accuracy, achieving the lowest MAE and MRE values and the highest R-squared value. This indicates that the ANN model provides more accurate predictions of polymer Tm compared to other models.

Table 4. Evaluation of Fuzzy Rules

2. Rule	3. MW Membership	4. Tg Membership	5. Hardness Membership
6. 1	7. Low (0.5)	8. Low (0.4)	9. High (0.4)
10. 2	11. Medium (0.5)	12. Medium (0.4)	13. Medium (0.5)
14. 3	15. High (0.1)	16. High (0.3)	17. Low (0.1)

Table 5. Membership and crisp values

Linguistic Term	Membership	Crisp Value
Low	0.4	20
Medium	0.5	50
High	0.1	80

Table 6. Model Performance Metrics

Model	*Mean Absolute Error*	*R-squared*	*Median Relative Error*
ANN	0.12	0.85	0.08
Random Forest	0.15	0.78	0.12
Support Vector Machine	0.18	0.72	0.15
Gradient Boosting	0.11	0.88	0.07

3.3.2. Comparison of Predicted Melting Temperature (Tm) Values by Machine Learning Models

The graphical representations serve as crucial tools in assessing the predictive capabilities of the model. (Figure 2), depicting the actual versus predicted melting temperature plot, showcases the model's alignment with observed data points, ideally clustering closely around the identity line for precise predictions. Additionally, (Figure 3), the residual plot, offers deeper insights into the model's performance by displaying the distribution of residuals.

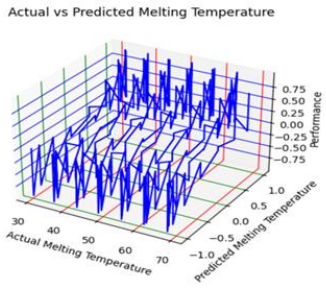

Figure 2. Actual Vs Predicted Melting Temperature

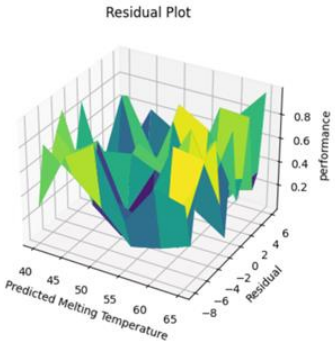

Figure 3. Residual Plot

3.4. Outputs of Polymer Genome Analysis

Polymer Genome is an advanced computational tool designed to facilitate the analysis, prediction, and optimization of polymer properties. Leveraging cutting-edge algorithms and machine learning techniques, Polymer Genome enables researchers and material scientists to explore the vast landscape of polymer chemistry with unprecedented efficiency and precision.

This work is applied for single polymer in polymer genome tool. Given Below are the property values for the polymer having SMILES notation

[*]=CC2CC(C=[*])C3CN(c1cc(C(F)(F)F)cc(C(F)(F)F)c1)CC23

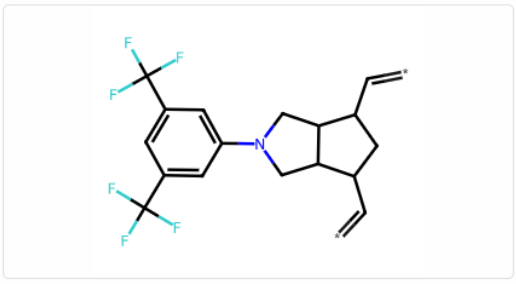

Figure 4. Polymer Structure

Table 7. Predicted Properties

Glass Transition Temperature	406K
Melting Temperature	584K
Thermal Decomposition Temperature	742K
Thermal Conductivity	0.19 W/mK
Tensile Strength	68 MPa
Young's Modulus	3 MPa

Proposed avenues for future research focus on refining the ANN model, addressing identified limitations, and expanding its scope to encompass a broader range of polymer systems and properties. By leveraging machine learning techniques and advanced computational methodologies, researchers can continue to push the boundaries of predictive modelling in polymer science, ultimately facilitating the design of novel materials with tailored properties and enhanced performance characteristics.

4. Conclusion

In this study, we explored the application of Artificial Neural Networks (ANN) in predicting the melting temperature (Tm) of polymers, offering a rapid and cost-effective alternative to traditional experimental methods. By training ANN models on parameters, molecular weight, glass transition temperature etc, we achieved accurate predictions of Tm. Our results underscored the effectiveness of convolutional layers for feature extraction from encoded monomer structures, coupled with optimization techniques such as customized loss functions and hyperparameter tuning, in enhancing model performance. The evaluation metrics provided comprehensive insights into the predictive accuracy of the ANN model, with graphical representations elucidating its capabilities and limitations. The ability of the model to capture intricate interactions between polymer structure and melting temperature was demonstrated by the residual analysis and the actual versus projected Tm plot. Furthermore, discussions highlighted the practical implications of our findings in materials science and engineering, emphasizing the potential of ANN models to guide materials design and development efforts. Moving forward, future research endeavours will focus on refining the ANN model, addressing inherent limitations, and expanding its applicability to diverse polymer systems and properties. By harnessing machine learning techniques and advanced computational methodologies, we aim to advance predictive modelling in polymer science, ultimately facilitating the design and synthesis of innovative materials with tailored properties and enhanced performance characteristics.

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