2023, 20(6 Suppl.): 2488-2497
https://dx.doi.org/10.21123/bsj.2023.8819
P-ISSN: 2078-8665 - E-ISSN: 2411-7986
Baghdad Science Journal

Processing of Polymers Stress Relaxation Curves Using Machine Learning Methods

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Received 29/03/2023, Revised 09/06/2023, Accepted 11/06/2023, Published 05/12/2023

Abstract

Currently, one of the topical areas of application of machine learning methods is the prediction of material characteristics. The aim of this work is to develop machine learning models for determining the rheological properties of polymers from experimental stress relaxation curves. The paper presents an overview of the main directions of metaheuristic approaches (local search, evolutionary algorithms) to solving combinatorial optimization problems. Metaheuristic algorithms for solving some important combinatorial optimization problems are described, with special emphasis on the construction of decision trees. A comparative analysis of algorithms for solving the regression problem in CatBoost Regressor has been carried out. The object of the study is the generated data sets obtained on the basis of theoretical stress relaxation curves. Tables of initial data for training models for all samples are presented, a statistical analysis of the characteristics of the initial data sets is carried out. The total number of numerical experiments for all samples was 346020 variations. When developing the models, CatBoost artificial intelligence methods were used, regularization methods (Weight Decay, Decoupled Weight Decay Regularization, Augmentation) were used to improve the accuracy of the model, and the Z-Score method was used to normalize the data. As a result of the study, intelligent models were developed to determine the rheological parameters of polymers included in the generalized non-linear Maxwell-Gurevich equation (initial relaxation viscosity, velocity modulus) using generated data sets for the EDT-10 epoxy binder as an example. Based on the results of testing the models, the quality of the models was assessed, graphs of forecasts for trainees and test samples, graphs of forecast errors were plotted. Intelligent models are based on the CatBoost algorithm and implemented in the Jupyter Notebook environment in Python. The constructed models have passed the quality assessment according to the following metrics: MAE, MSE, RMSE, MAPE. The maximum value of model error predictions was 0.86 for the MAPE metric, and the minimum value of model error predictions was 0.001 for the MSE metric. Model performance estimates obtained during testing are valid.

Keywords: Artificial intelligence, CatBoost, Machine learning, Metaheuristics, Polymers, Regularization, Regression, Rheology.

Introduction

Currently, polymeric materials and composites based on them are increasingly used in construction and other industries. As with traditional building materials such as wood and concrete, polymeric materials are characterized by a pronounced creep phenomenon. Solving the problem of polymer mechanics is impossible without determining their rheological properties. The rheological behavior of

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polymeric materials can be described by linear[1] and nonlinear models[2-5]. Nonlinear models are more complex, but at the same time provide better agreement with experimental data. One of the simplest linear models is the Maxwell-Thompson model, in which the body is represented as a combination of viscous and elastic elements. Introduction to this model by G.I. Gurevich, the dependence of the relaxation viscosity of the polymer on stress made it possible to obtain good agreement with experiment for many polymers[6–9]. In the case of a uniaxial stress state, the basic Eq. of the Maxwell-Gurevich model has the form[10]:

$$\frac{\partial \varepsilon^*}{\partial t} = \frac{f^*}{\eta^*} \quad 1$$

$$f^* = \sigma - E_\infty \varepsilon^* \quad 2$$

$$\frac{1}{\eta^*} = \frac{1}{\eta_0^*} \exp\left(\frac{|f^*|}{m^*}\right) \quad 3$$

In Eq. 1-3 ε^* is the creep strain, f^* is the stress function, σ is the stress, E_∞ is the high elasticity modulus, η_0^* is the initial relaxation viscosity (hereinafter simply "viscosity"), m^* is the velocity modulus.

The modulus of high elasticity is a relaxation constant that establishes a relationship between the ultimate creep strain at $(t \to \infty)$ and the applied stress $E_\infty = \sigma_\infty / \varepsilon_\infty^*$. The determination of this value is carried out from experiments on creep or stress relaxation and is not difficult if the experimental curve reaches a horizontal asymptote. Finding the quantities m^* and η_0^* at the same time is associated with certain difficulties, since the theoretical creep and relaxation curves using the Maxwell-Gurevich equation cannot be described by analytical functions. Some algorithms for determining these quantities are presented in papers [11-13]. The disadvantage of these algorithms is the high quality requirements for experimental curves.

Artificial intelligence methods have great prospects in the problems of determining the properties of materials, including polymers. The paper[14] was the first to present a technique for processing polymer relaxation curves using artificial neural networks (ANNs). In addition to ANN, efficient machine learning algorithms include the CatBoost Regressor (Adaptive Boosting) algorithm. Adaptive Boosting (AdaBoost) is a high-level metaheuristic belonging to the class of combined optimization methods that organizes a direct random search for probable solutions that are optimal or close to optimal solutions until a given condition is met or a given number of iterations is reached. Combinatorial optimization algorithms allow solving a large number of practical problems, such as, for example, the traveling salesman problem, assignment problems, scheduling problems, building decision trees, the dimension of which can reach exponential. The authors of the articles[15-17] offer an overview of the main directions of metaheuristic approaches (local search, evolutionary algorithms) to solving combinatorial optimization problems. Metaheuristic algorithms in optimal content search problems have a wide range of tasks, including tasks related to model training, are an alternative solution for deep learning of a neural network, and solve the problems of model retraining[16].

When choosing families of algorithms for solving a regression problem in CatBoost Regressor, the choice is often left in favor of decision trees, although these may be linear algorithms or some others.

Frequently occurring patterns in the training sample, which cannot but be present in the test sample, can negatively affect the test sample or the entire sample of the training space, which leads the model to overfitting. In other words, such regularities have the character of coincidence. The more degrees of freedom our model has, the more risks there are in overfitting.

So, for example, in models built on decision tree algorithms, retraining occurs quite quickly on simple models, when building a decision tree with a large depth, retraining can be avoided and the ideal quality of the model can be achieved, only because each element of the training sample will have its own leaf in the decision tree.

Further, a very clear example is the k-nearest neighbors algorithm, which adjusts to the training sample, since, among the k-nearest neighbors of the object under consideration, there may be an outlier or conditionally local noise that will lead to an error in the entire algorithm.

Linear algorithms are prone to overfitting, because for them it is necessary to take into account the dimension of features, if the dimension of features from the number of features is much larger, then retraining is inevitable, because there will be too many degrees of freedom for a small sample size.

Of course, overfitting models is a common practice when testing them, when there is at least some decision condition in the context of incomplete or sparse data, however, in practice, in the context of machine learning, overfitting is understood as a

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significant deviation in the quality of the training set model from the test set.

The purpose of this article is to build a model for predicting the rheological parameters of a polymer from stress relaxation curves based on the Adaptive Boosting algorithm.

Materials and Methods

The technique for processing stress relaxation curves was tested on the example of the epoxy binder EDT-10, which acts as a polymer matrix in glass-reinforced plastics. To train the model, three data sets were generated according to the method given in[14], with different dataset dimensions. The datasets contain 5 input parameters:

1. The strain value ε at which the stress relaxation experiment is carried out;
2. The stress at the initial time σ_0;
3. The stress at the end of the relaxation process (at $t \to \infty$);
4. The relaxation time;
5. The conditional end time of the process (the time when the difference between the current stress and the stress at $t \to \infty$ does not exceed 5%).

Based on five input parameters taken from the experimental stress relaxation curve, the model should predict the velocity modulus and relaxation viscosity. Tables 1 - 3 partially present the analyzed data arrays. The total number of numerical experiments was: n_1 = 102900; n_2 = 107520; n_3 = 180000. Fragments of initial data for the model training are shown in Tables 1-3.

Table 1. Table of initial data for model training (n_1)

No	Strain, %	Stress at the initial moment, MPa	Stress at the end of the process, MPa	Relaxation time, hours	Conditional end time of the process, hours	Velocity module, MPa	Viscosity, 106 MPa·s
1	1	20	6.666666667	0.00259842	0.273543249	2	5
2	2	40	13.33333333	3.60E-05	0.110365845	2	5
3	3	60	20	6.30E-07	0.051685264	2	5
4	1	20	6.666666667	0.08131234	8.559969561	2	156.4646
5	2	40	13.33333333	0.00112781	3.453670584	2	156.4646
6	3	60	20	1.97E-05	1.617383311	2	156.4646
7	1	20	6.666666667	0.00259842	0.273543249	2	5
…							
102897	3	120	60	0.000701874	46.05477107	4	14848.53
102898	1	40	20	2.923228748	307.7361555	4	15000
102899	2	80	40	0.040545747	124.1615756	4	15000
102900	3	120	60	0.000709034	46.52455947	4	15000

Table 2. Table of initial data for model training (n_2)

No	Strain, %	Stress at the initial moment, MPa	Stress at the end of the process, MPa	Relaxation time, hours	Conditional end time of the process, hours	Velocity module, MPa	Viscosity, 106 MPa·s
1	1	20	6.666666667	0.00259842	0.273543249	2	5
2	2	40	13.33333333	3.60E-05	0.110365845	2	5
3	3	60	20	6.30E-07	0.051685264	2	5
4	1	20	6.666666667	0.11553579	12.16276361	2	222.3188406
5	2	40	13.33333333	0.00160250	4.90728134	2	222.3188406
6	3	60	20	2.80E-05	2.298121593	2	222.3188406
7	1	20	6.666666667	0.00259842	0.273543249	2	5
…							
107517	3	120	60	0.00069876	45.85051525	4	14782.68116
107518	1	40	20	2.92322874	307.7361555	4	15000
107519	2	80	40	0.04054574	124.1615756	4	15000
107520	3	120	60	0.00070903	46.52455947	4	15000

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P-ISSN: 2078-8665 - E-ISSN: 2411-7986
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Table 3. Table of initial data for model training (n_3)

No	Strain, %	Stress at the initial moment, MPa	Stress at the end of the process, MPa	Relaxation time, hours	Conditional end time of the process, hours	Velocity module, MPa	Viscosity, 106 MPa·s
1	1	20	6.666666667	0.002598426	0.273543249	2	5
2	2	40	13.33333333	3.60E-05	0.110365845	2	5
3	3	60	20	6.30E-07	0.051685264	2	5
4	1	20	6.666666667	0.134677718	14.1778857	2	259.15254
5	2	40	13.33333333	0.001868006	5.720317864	2	259.15254
6	3	60	20	3.27E-05	2.678873513	2	259.15254
7	1	20	6.666666667	0.002598426	0.273543249	2	5
…							
179997	3	120	60	0.00069702	45.73627046	4	14745.847
179998	1	40	20	2.923228748	307.7361555	4	15000
179999	2	80	40	0.040545747	124.1615756	4	15000
180000	3	120	60	0.000709034	46.52455947	4	15000

Tables 4 - 6 present the statistical characteristics of the initial data sets by samples n_1, n_2, n_3 respectively.

Table 4. Statistical characteristics of the original data set (n_1)

Parameter	Strain	Stress at the beginning of the process	Stress at the end of the process	Relaxation time	Conditional end time of the process	Velocity modulus	Viscosity
Units	%	MPa	MPa	hours	hours	MPa	106 MPa·s
count	102900.00	102900.00	102900.00	102900.00	102900.00	102900.00	102900.00
mean	2.00	60.0	25.40	1.92	144.38	3.00	7502.50
std	0.82	28.42	12.58	6.07	175.42	0.67	4372.21
min	1.00	20.00	6.67	0.00	0.00	2.00	5.00
max	3.00	120.0	60.00	83.66	1504.03	4.00	15000.00

Table 5. Statistical characteristics of the original data set (n_2)

Parameter	Strain	Stress at the beginning of the process	Stress at the end of the process	Relaxation time	Conditional end time of the process	Velocity modulus	Viscosity
Units	%	MPa	MPa	hours	hours	MPa	106 MPa·s
count	107520.00	107520.00	107520.00	107520.00	107520.00	107520.00	107520.00
mean	2.00	60.00	25.41	1.87	140.67	3.00	7502.50
std	0.82	28.28	12.51	5.87	171.28	0.65	4390.99
min	1.00	20.00	6.67	0.00	0.00	2.00	5.00
max	3.00	120.00	60.00	83.66	1504.03	4.00	15000.00

Table 6. Statistical characteristics of the original data set (n_3)

Parameter	Strain	Stress at the beginning of the process	Stress at the end of the process	Relaxation time	Conditional end time of the process	Velocity modulus	Viscosity
Units	%	MPa	MPa	hours	hours	MPa	106 MPa·s
count	180000.00	180000.00	180000.00	180000.00	180000.00	180000.00	180000.00
mean	2.00	60.00	25.42	1.80	139.77	3.00	7502.50
std	0.82	28.11	12.42	5.60	167.00	0.64	4401.45

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min	1.00	20.00	6.67	0.00	0.00	2.00	5.00
max	3.00	120.00	60.00	83.66	1504.03	4.00	15000.00

One of the ways to deal with overfitting of the model is the regularization of the loss function, due to the regularization coefficients that specify the redistribution of weights in the model, the loss function takes a minimum value. This method provides improved model accuracy and reduces unnecessary deviations.

Regularization through the loss function in deep learning implies the use of the weight decay method (Weight Decay), in which the regularization coefficients λ(i) avoid the entropy of the distribution of neural network predictions. Regularization is performed according to Eq. 4:

$$L_r(i+1) = L_r(i) + \lambda(i)W(i) \qquad 4$$

where i is the serial number of the current iteration; $W(i)$ is the norm of the weight vector; $L_r(i+1)$ is the regularization function.

Each neural network weight is updated proportionally according to the gradient of the loss function. This method was combined with the Adam gradient descent method, as a result of a combination of the optimization method and the regularization technique through the loss function, the AdamW method appeared[17].

Another option to combat model overfitting is cross-validation. In this method, the model is trained k times, instead of once, as provided in the loss function regularization method. The idea is as follows, according to the scheme in Fig. 1: on each experiment, the k-th window (validation block) is selected from k elements; on the rest k-1 windows, training takes place and then the quality of the model is checked. Thus, patterns formed earlier are destroyed and new, better ones are formed, until the model error becomes digestible. This method has already been used by authors in paper[18] and observed in the works of other scientists[19].

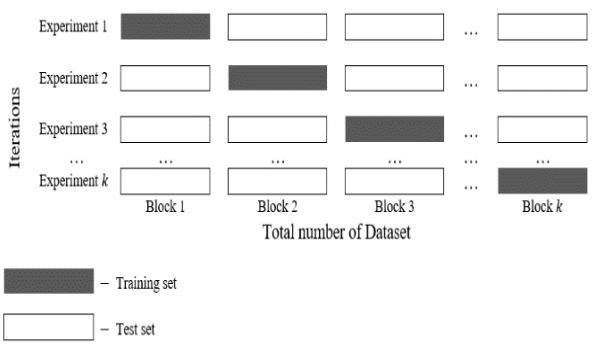

Figure 1. Splitting data into *k*-block cross-validation

The third way to regularize a neural network is to change the data. Data augmentation implies the addition of data, for example, with dispersion noise, by increasing the size of the training sample, new data can improve the quality of the model, increase its sensitivity and robustness. Having received additional data, the neural network understands which transformations over them are valid. Most often, data augmentation is used in the field of computer vision.

In this paper, the focus will be made on the second method of data regularization, namely, related to changing the network structure.

When building a predictive model, it is important to determine the function that evaluates the quality of this model. To assess the quality of the functioning of a neural network when solving a regression problem, it is enough to use two functions RMSE and MAPE, in contrast to classification tasks, where functions such as MSE and MAE are additionally used. In our work, the predictive capabilities of the built models will be evaluated on different samples and compared with the results obtained for models built with different parameters. Table 7 presents the metrics used in the work and shows their advantages and disadvantages. The coefficient of determination (R^2) is calculated by the Eq. 5:

$$R^2 = \frac{\left(\sum_{t=1}^{T}(y_t - \bar{y}_t)(\hat{y}_t - \bar{\hat{y}}_t)\right)^2}{\sum_{t=1}^{T}(y_t - \bar{y}_t)^2 \sum_{t=1}^{T}\left(\hat{y}_t - \bar{\hat{y}}_t\right)^2} \qquad 5$$

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https://dx.doi.org/10.21123/bsj.2023.8819
P-ISSN: 2078-8665 - E-ISSN: 2411-7986
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Table 7. Quality Metrics for Analyzing Regression Models

Quality Metric	Formula	Advantages	Disadvantages
Mean Absolute Error (MAE)	$MAE = \frac{1}{T}\sum_{t=1}^{T}\lvert y_t - \hat{y}_t\rvert$	More robust model estimation than RMSE. Unaffected by emissions. Almost corresponds to the median.	Difficult to interpret. It is possible to compare estimates for only one data set.
Mean Squared Error (MSE)	$MSE = \frac{1}{T}\sum_{t=1}^{n}(y_t - \hat{y}_t)^2$	It is possible to compare models on different samples.	Affected by outliers.
Root-Mean-Square Error (RMSE)	$RMSE = \sqrt{\frac{1}{T}\sum_{t=1}^{T}(y_t - \hat{y}_t)^2}$	It is used both in predicting positive and negative values.	Unsteady estimate, uses average values.
Mean Absolute Percentage Error (MAPE)	$MAPE = \frac{1}{T}\sum_{i=1}^{T}\left\lvert\frac{y_t - \hat{y}_t}{\hat{y}_t}\right\rvert 100$	It is an effective criterion for evaluating the coefficients of models.	It is possible to compare estimates for only one data set.

Results and discussion

In this section, we will present the prediction results based on three datasets. Training of CatBoost Regressor (XGBRegressor) models was carried out according to the following scheme. The depth of the tree was adjusted according to the values: {4,6,8,10}; learning rate: {0.01, 0.03, 0.05, 0.07, 0.08, 0.09} number of iterations: {500, 800, 1000, 1500}; coefficient in Eq. 4 $\lambda(i) = 3$ to achieve the smallest prediction error. Table 8 shows the sets of the best values of the parameters of the CatBoost Regressor models by samples $n_1;n_2;n_3$ for the parameters: "Viscosity" (η_0^*: $\eta_{01}^*;\eta_{02}^*;\ \eta_{03}^*$); "Velocity module" ($m^*$: $m_1^*;\ m_2^*;\ m_3^*$) respectively.

Table 8. Best Parameter Values for CatBoost Regressor Models

Parameter	Tree depth	Learning rate	Number of iterations
η_{01}^*	6	0.08	1000
m_1^*	6	0.08	800
η_{02}^*	6	0.08	1000
m_2^*	6	0.08	800
η_{03}^*	6	0.08	1000
m_3^*	6	0.08	800

According to Table. 8, frequent coincidences of the best values of the parameters on different samples can be observed. This is due to the fact that the statistical characteristics of the original data sets described earlier in some cases coincide, or vary in the range from 10^{-1} to 10^{-3}. In particular, the same values of model training parameters for three data sets are because each of them describes processes that are identical in nature.

The loss function and the forecast accuracy of the model are stabilized in the mode of 800 iterations for the parameter m^*, and 1000 iterations for the parameter η_0^* for all models at the training stage.

Qualitative estimation of model parameters is as follows. For the parameter η_0^*: η_{01}^* – RMSE = 0.08; R2 = 0.993; η_{02}^* – RMSE = 0.08; R2 = 0.994; η_{03}^* – RMSE = 0.10; R2 = 0.989. For the parameter m^*: m_1^* – RMSE = 0.05; R2 = 0.998; m_2^* – RMSE = 0.05; R2 = 0.997; m_3^* – RMSE = 0.06; R2 = 0.997.

The disadvantage of this method is that it incurs a considerable amount of time, since the algorithm for finding the optimal parameters over the grid is very slow due to the potentially large number of combinations being tested. Given all combinations of model parameter values, each model was trained for at least 480 epochs. To obtain the resulting model, the early stopping method was applied. The AdamW method was used as an optimization method. The performance metrics of the algorithm are given in Table 9.

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https://dx.doi.org/10.21123/bsj.2023.8819
P-ISSN: 2078-8665 - E-ISSN: 2411-7986
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Table 9. Algorithm Performance Metrics

Parameter	MAE	MSE	RMSE	MAPE (%)	R2train	R2test
η_{01}^*	0.06	0.01	0.08	0.43	0.99386	0.99344
m_1^*	0.03	0.001	0.05	0.08	0.99751	0.99713
η_{02}^*	0.06	1.01	0.08	0.20	0.99448	0.99413
m_2^*	0.04	0.001	0.05	0.08	0.99765	0.99725
η_{03}^*	0.08	0.01	0.10	0.86	0.98965	0.98917
m_3^*	0.04	0.001	0.06	0.11	0.99670	0.99650

Fig. 2 - 4 show the prediction graphs for training samples (dotted line), test samples (solid line) of final models with the best parameters according to Table 8, for η_0^* (a); m^* (b) by samples $n_1; n_2; n_3$ according to designations.

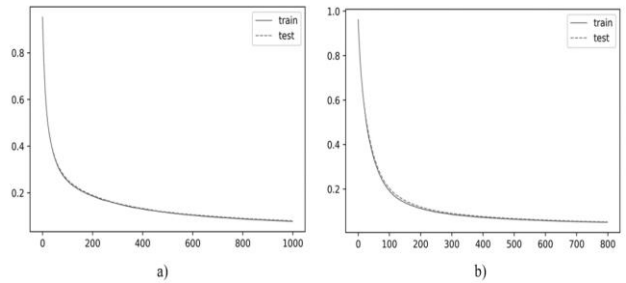

Figure 2. Forecast plots on the sample (n_1) by parameters

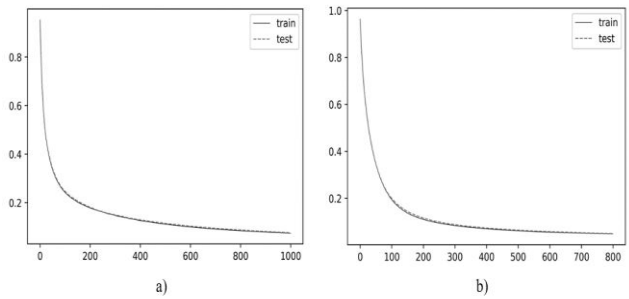

Figure 3. Forecast plots on the sample (n_2) by parameters

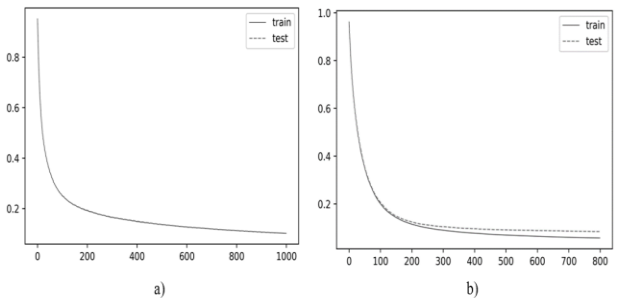

Figure 3. Forecast plots on the sample (n_3) by parameters

The relationship between actual and predicted values for parameters: η_0^* (a); m^* (b) are shown in Fig. 5 – 7 by samples $n_1; n_2; n_3$ according to designations.

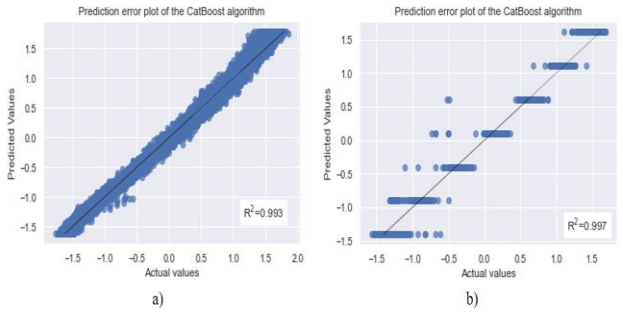

Figure 4. Plots of forecast errors (n_1)

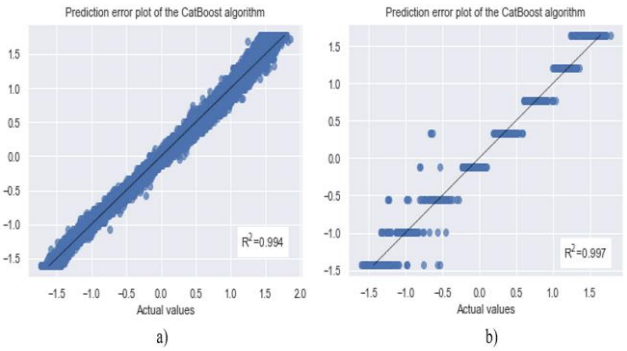

Figure 5. Plots of forecast errors (n_2)

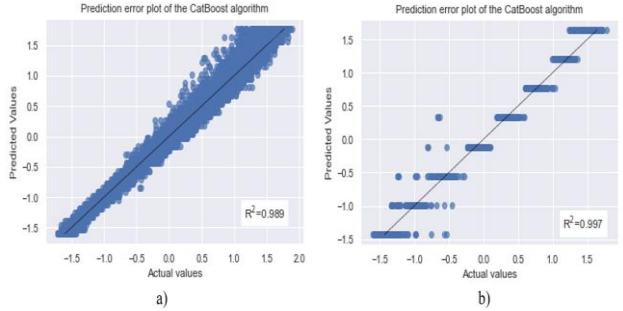

Figure 6. Plots of forecast errors (n_3)

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https://dx.doi.org/10.21123/bsj.2023.8819
P-ISSN: 2078-8665 - E-ISSN: 2411-7986
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The forecast error plots show the actual values from the dataset versus the predicted values generated by our model. This visualization method allows one to see how large the variance is in the model.

Conclusion

Artificial intelligence methods are successfully applied in various industries, for example, in the construction process at all stages, including quality control in the production of building materials, including polymeric materials and composites based on them. Intelligent models built on the basis of CatBoost were implemented in the Jupyter Notebook environment in Python. The training involved the generated data sets obtained by constructing theoretical stress relaxation curves using the Euler method on the example of the EDT-10 epoxy binder. For the developed intelligent models of the rheological parameters of polymers (initial relaxation viscosity, velocity modulus), the quality of the models was assessed, prediction graphs were plotted for trainees and test samples, including error prediction graphs for the final models with the best parameters.

Taking into account the fact that the developed machine learning algorithms were applied on a large amount of data depending on a large number of parameters, there is always a data error that is within 10%. In our case, the value of the MAPE metric obtained when testing the developed machine learning models is acceptable and represents the range of 0.08 - 0.86. Thus, models can be verified and accepted for use in determining the rheological parameters of polymers.

In the future, further research is planned to expand the range of tools and methods of machine learning, such as k-nearest neighbors, support vector regression (SVR).

Acknowledgment

The authors would like to acknowledge the administration of Don State Technical University for their resources and financial support.

Author's Declaration

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are ours. Besides, the Figures and Images, which are not ours, have been given the permission for re-publication attached with the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee in Don State Technical University.

Authors' Contributions Statement

This work was carried out in collaboration between all authors. The datasets for models training were generated by A.C. Machine learning models were developed by T.K. and E.A. T.K. wrote and edited manuscript with revisions idea. A.C. and E.A. analyzed the data with revisions idea. All authors read and approved the final manuscript.

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2023, 20(6 Suppl.): 2488-2497
https://dx.doi.org/10.21123/bsj.2023.8819
P-ISSN: 2078-8665 - E-ISSN: 2411-7986
Baghdad Science Journal

معالجة منحنيات استرخاء الإجهاد للبوليمرات بطرق التعلم الآلي

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الخلاصة

حاليًا، أحد المجالات الموضوعية لتطبيق طرق التعلم الآلي هو التنبؤ بالخصائص المادية. الهدف من هذا العمل هو تطوير نماذج التعلم الآلي لتحديد الخصائص الريولوجية للبوليمرات من منحنيات استرخاء الإجهاد التجريبية. تقدم الورقة لمحة عامة عن الاتجاهات الرئيسية للنهج الميتاهويرية (البحث المحلي، والخوارزميات التطورية) لحل مشاكل التحسين التوافقي. يتم وصف الخوارزميات الميتاهورية لحل بعض مشاكل تحسين التوافقية المهمة، مع التركيز بشكل خاص على بناء أشجار القرار. تم إجراء تحليل مقارن للخوارزميات لحل مشكلة الانحدار في CatBoost Regressor. الهدف من الدراسة هو مجموعات البيانات المتولدة التي تم الحصول عليها على أساس منحنيات استرخاء الإجهاد النظرية. وترد جداول البيانات الأولية لنماذج التدريب لجميع العينات، ويجري تحليل إحصائي لخصائص مجموعات البيانات الأولية. كان العدد الإجمالي للتجارب العددية لجميع العينات 346020 اختلافًا. عند تطوير النماذج، تم استخدام طرق CatBoost للذكاء الاصطناعي، وتم استخدام طرق التسوية (تحلل الوزن، وتسوية الوزن المفصول، وزيادة) لتحسين دقة النموذج، وتم استخدام طريقة Z-Scoreلتطبيع البيانات. نتيجة للدراسة، تم تطوير نماذج ذكية لتحديد المعلمات الريولوجية للبوليمرات المدرجة في معادلة ماكسويل-غوريفيتش غير الخطية المعممة (لزوجة الاسترخاء الأولية، وحدة السرعة) باستخدام مجموعات البيانات المولدة لرابط الإيبوكسي-EDT 10كمثال. بناءً على نتائج اختبار النماذج، تم تقييم جودة النماذج، ورسم رسوم بيانية للتنبؤات للمتدربين وعينات الاختبار، ورسوم بيانية لأخطاء التنبؤ. تستند النماذج الذكية إلى خوارزمية CatBoost ويتم تنفيذها في بيئة دفتر المشتري في بايثون. اجتازت النماذج المشيدة تقييم الجودة وفقًا للمقاييس التالية MAE :و MSE و RMSE و MAPE. كانت القيمة القصوى لتنبؤات خطأ النموذج 0.86 لمقياسMAPE ، والقيمة الدنيا لتنبؤات خطأ النموذج كانت 0.001 لمقياس MSE.
تقديرات أداء النموذج التي تم الحصول عليها أثناء الاختبار.

الكلمات المفتاحية : الذكاء الاصطناعي، **CatBoost** ، التعلم الآلي، ميتاهوريستيكش، البوليمرات، التسوية، الانحدار، الريولوجيا.