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Research article

Fine-tuning optimization of poly lactic acid impact strength with variation of plasticizer using simple supervised machine learning methods

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Abstract. The use of machine learning to fine-tune the properties of materials is a remarkable achievement in the 21st century. Three machine learning (ML) methods were used to fine-tune and optimize the impact strength of polylactic acid (PLA) with different plasticizers: KNN (K-nearest neighbors), SVR (Support Vector Regression), and ANN (artificial neural networks). The results demonstrated that, though ANN reached a higher R^2 score of 0.901 than the other two ML methods, KNN, with an R^2 score of 0.839, showed more stability than ANN. Based on the current research, KNN is recommended for experimentalists to fine-tune the impact strength of variational plasticizers. The experiment study case with polyethylene glycol 1000 (PEG1000) and octyl epoxy stearate (OES) plasticizer showed good agreement and prediction with experiments. It even showed the fine-tuned impact strength as a function of plasticizer content results, which cannot be achieved by only experiments.

Keywords: *biodegradable polymers, mechanical properties, modelling and simulation*

1. Introduction

Polylactic acid (PLA) is a biopolymer material that has a high potential to be developed due to particular properties such as degradability, biocompatibility, good processability, and relatively good mechanical properties in comparison to other biopolymers [1–3]. The increasing attention to climate change and global warming makes PLA an alternative material in the plastics industry [4]. However, despite its advantages in comparison to petroleum-based polymers, PLA is relatively brittle, stiff, and has low impact strength [5]. These deficiencies make the use of PLA limited to short-term or merely disposable products [6]. The insufficient impact strength of PLA limits its application to broader uses, such as electronic device housing and so on [7]. The use of plasticizers is one

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of the methods to modify PLA's impact strength [8]. However, owing to the wide variety of plasticizer types, it is challenging to select appropriate plasticizers to obtain the specific values of impact strength and optimize them. The trial-and-error experiments require a lot of costs and time, thus rendering these methods ineffective.

The use of machine learning (ML) to guide plastics engineers to find new types of materials is increasingly common, for example, Kim *et al*. [9] used a genetic algorithm (GA) in tandem with ML to design polymer with specific glass transition temperature and high bandgap. The advantage of using GA with ML is that they require less number of hyperparameters than other generative models. In addition, there have been many efforts to optimize specific properties of polymers and polymer composites, such as dielectric properties using kernel ridge regression (KRR) [10] and the least absolute shrinkage and selection operator (LASSO) method [11], glass temperature using active learning [12], gas permeabilities using gaussian process regression [13], mechanical properties using artificial neural networks (ANN) [14] and convolutional neural networks (CNN) [15], and to design smart, self-sensing fiber reinforced plastics using ANN [16]. However, most of these efforts described are too complicated to be useful for ordinary users, and some require large databases for example ANN.

Lukasiak *et al*. [17] employed KNN to recognize a pattern of polymeric materials. Tapkin *et al*. [18] used a simple machine-learning method of K-nearest neighbors (KNN) and support vector machine (SVM) to classify Bitumen Images and use them for polypropylene concentration prediction. Costa *et al*. [19] and Gajarska *et al*. [20] used KNN to classify of polymer e-waste and twenty polymers respectively by means of laser-induced breakdown spectroscopy (LIBS). However, KNN and SVM were largely used in classification or pattern recognition.

In this paper, the impact strength of plasticized PLA is predicted and optimized using simple machine learning methods: support vector regression (SVR), KNN, and ANN with a relatively small database. The reason for using these methods is that they are simple and can be used even by beginner industrial users. The use of SVR and KNN is for representative simple supervised ML models, while ANN is for complex ones. ANN is one of the most common methods in the deep learning regime, albeit still the simplest. The other reason is the limitation of data. It is well known that SVR and KNN are suitable for small sets of data but these methods will easily lead to overfitting. Thus, it needs to be compared with the ANN model which is suitable for a large data set, however according to Feng *et al*. [21] fine-tuned deep neural network (DNN) shows better generalization performance in comparison to simple supervised ML methods.

This study does not use inverse design to select new materials, instead using simple experiments to validate and select specific plasticizer types based on optimized ML methods. The advantage of our approach is that it is simple and can be used by an ordinary user or plastics engineer to optimize their material selection.

2. Methods

2.1. Dataset characteristics

The prediction of plasticized PLA impact strength involves a dataset containing data from previous experiments with information on the PLA matrix and plasticizer properties. After sorting, cleaning, and trimming the data samples, a total of 54 samples were collected from 11 different previous experiments, which consisted of 14 different types of plasticizers with content in the range of 1 to 30% that were melt-blended with PLA (molecular weight in the range of 86 170 to 207 000 g/mol). The input parameters used for prediction are PLA molecular weight, plasticizer molecular weight, plasticizer density, as well as plasticizer content, and the parameter to be predicted is mechanical impact strength. Statistical information for this dataset is shown in Table 1. Plasticizer content measures the weight ratio of plasticizer to PLA.

Table 1. Statistical information of the plasticized PLA dataset.

No.	Features		Mean	Minimum	Maximum	Standard deviation
1.	PLA molecular weight	[kg·mol^{-1}]	137.08	86.17	207.00	44.81
2.	Plasticizer molecular weight	[kg·mol^{-1}]	0.80	0.16	1.37	0.42
3.	Plasticizer density	[g·cm^{-3}]	1.03	0.90	1.30	0.12
4.	Plasticizer content	[wt%]	11.00	1.00	30.00	6.87
5.	Impact strength	[kJ·m^{-2}]	29.98	4.80	62.90	14.48

2.2. Machine learning models

In this paper, we use SVR, KNN, and ANN to predict plasticized PLA impact strength which is programmed using Python programming language version 3.8. SVR and KNN are the classic and simplest shallow ML methods and can be easily understood by plastics engineers and experimentalists. Both methods are on the extreme end of the spectrum of shallow ML methods. SVR requires a minimal number of tuning parameters and can be used properly with careful feature selection, while KNN has a lot of tuning parameters but is also sensitive to outliers. We realize that in polymer science, outlier data exist due to many unknown or hidden experiment settings. The development of the KNN and SVR models is done by using the Scikit-learn Python library. The KNN model involves K parameters, which describe the number of closest data points to be taken as a representation of the data points to be predicted. The predicted result of the KNN model is the average of the output of the closest data points, as shown in Equation (1):

$$\hat{y}(x) = \frac{1}{k}\sum_{x_i \in N_{k(x)}} y_i \tag{1}$$

where $\hat{y}(x)$ is the predicted result, k denotes the number of closest data points to the input data x, and y_i represents the labels of those data points [22]. Euclidean distance was used as the distance calculation metric since it is the default and widely used metric in KNN, as well as generally works great on low-dimensional numeric data compared to other metrics. Euclidean distance calculation can be performed using Equation (2) below:

$$d(p,q) = d(q,p) = \sqrt{\sum_{i=1}^{n}(q_i - p_i)^2} \tag{2}$$

where $d(p,q)$ is the Euclidean distance between two points of q and p.

The SVR model is built using the radial basis function (RBF) kernel and includes C and gamma parameters. The kernel is a function that is useful for projecting low-dimensional original data to higher dimensions, as well as converting SVR model computing systems from linear to non-linear and having different mapping capabilities, which can affect the performance of the SVR model. RBF is one of the kernels in SVR that can be used for almost all types of data and involves the gamma parameter, which describes the magnitude of the influence distance from a data point, thus affecting the degree of curvature of the line or plane defined by the model [23]. The gamma (γ) value is determined by the RBF kernel free parameter value (σ), which is expressed through Equation (3) below:

$$\gamma = \frac{1}{2\sigma^2} \tag{3}$$

Unlike the gamma parameter, parameter C is a penalty factor, which can be used for all types of kernels to balance empirical risk and model confidence level. Parameter C affects how much deviation the SVR model can tolerate, which is directly correlated with the slack variable (ξ) [24], as shown by Equation (4):

$$T = \min:\frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\left(\xi_i - \xi_i^*\right) \tag{4}$$

where T is the SVR goal to minimize the function on the right-hand side of the equation, w is weight, and is the penalty parameter.

The ANN model is built using the TensorFlow library and involves parameters such as the number of hidden layers and the number of nodes in each layer, epoch, batch size, and learning rate. Epoch describes the model training cycle against all data in the training dataset. The batch size describes the amount of data that will be passed into the ANN model at one time, while the learning rate describes how fast the ANN model learns by determining the weight adjustments to the model based on the gradient loss for each epoch. When it comes to training the model using the data set, each of those models has its own way of interpreting the data, thus resulting in different capabilities and limitations. The advantages and disadvantages of using these models are explained in Table 2. The data set will be fed into each model to see which model can handle the data well based on their superiorities and limitations.

2.3. Prediction performance evaluation

The performance of these models in predicting plasticized PLA impact strength was known by calculating the R^2 score, root mean square error (*RMSE*), and relative root mean square error (*RRMSE*). The R^2 score is an evaluation metric that represents the magnitude of the difference between the model's predicted value and the actual value in the dataset, which is calculated based on Equation (5):

Table 2. The advantages and disadvantages of KNN, SVR, and ANN models [25–30].

KNN		SVR		ANN	
Advantage	**Disadvantage**	**Advantage**	**Disadvantage**	**Advantage**	**Disadvantage**
• No training period. • Easy to implement. • Has few parameters to set. • Gives good results even if there is not enough information about the data (few data).	• Does not work well with large data sets and high-dimensionality. • Sensitive to noise and missing data. • To work properly, the features must be expressed in the same scale.	• Generally works well in high-dimensional spaces. • Robust to outliers. • Easy to implement. • Has few parameters to set.	• Not suitable for large data sets. • May be difficult to interpret and understand. • Does not work well when the number of features exceeds the number of training data.	• Can be applied to complex non-linear problems. • Works well with large data sets. • Provides quick predictions after training.	• Has many parameters to set. • Computations are difficult and time-consuming. • Weights and biases are initialized randomly, making the resulting predictions inconsistent.

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2} \quad (5)$$

where n, y, $\bar{y}_i$, dan $\hat{y}_i$ are the sum of the data, the actual value, the average value, and the model's predicted value, respectively. The R^2 score value is in the range –∞ to 1, where the level of accuracy will be higher if the value is close to 1 [31]. Meanwhile, *RMSE* is an evaluation metric that measures the standard deviation of the prediction error, represented by the square root of the average difference in the model's predicted value and the actual value, which is calculated using Equation (6) below:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2} \quad (6)$$

The *RMSE* value is in the range of 0 to +∞, where the level of accuracy will be higher if the value is closer to 0, indicating the closer the distance between the predicted value and the actual value [32].

A dimensionless variant of *RMSE* is *RRMSE*. *RRMSE* is a measure of root mean square error that has been scaled against the actual value and then normalized by the root mean square value. *RRMSE* may be used to compare various measurement techniques, whereas *RMSE* is constrained by the original measurements' scale. An increased *RRMSE* happens when the predictions turn out to be wrong. *RRMSE* expresses the error as a percentage or relative and the value is calculated using Equation (7):

$$RRMSE = \sqrt{\frac{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y})^2}{\sum_{i=1}^{n}(y_i)^2}} \quad (7)$$

2.4. Experimental design

Validation of the machine learning model prediction results was also carried out through experiments. The same impact resistance experiments as Sungsanit *et al*. [33] and Ferri *et al*. [34] were re-conducted, involving samples in the form of polyethylene glycol (PEG) and octyl epoxy stearate (OES) plasticized PLA. PLA was obtained from Repreper Tech Co., Ltd (Kowloon, Hong Kong) in the form of plastic pellets, PEG1000 (molecular weight of 1000 g·mol^{-1}) was obtained from Merck (Darmstadt, Germany), and OES (molecular weight of 408 g·mol^{-1}) was obtained from Traquisa (Barcelona, Spain). Mixing of dried PLA and PEG1000 (with content variations of 5, 10, 15, and 20 wt%) was done in a rheomixer at a temperature of 190 °C and a stirring speed of 30 rpm for 15 minutes, while dried PLA and OES (with content variations of 1, 3, 5, 10, 15 and 20 wt%) were mixed at a temperature of 180 °C and a stirring speed of 60 rpm. The impact resistance testing was carried out at room temperature using the Izod method, according to the ASTM D256 standard specification. The 2.5 millimeters-depth notched specimens with the size of 64×12.7×3.2 mm were injection molded and were dried in the vacuum oven overnight prior to testing. The test was performed using a Davenport impact tester with a pendulum hammer of 1.36 J.

3. Results and discussions

3.1. KNN model performance

Three ML algorithms were used: KNN, SVR, and ANN. The parameters of these algorithms were optimized to obtain the best R^2 score. First, the KNN algorithm was built to do prediction with a variation of the K parameter which shows the number of nearest neighbors. KNN uses the distance between data

Table 3. Effect of variations in *K* values on KNN performance.

K	R^2 score	*RMSE*	*RRMSE*
1	0.839	0.080	15.327
2	0.583	0.129	24.667
3	0.428	0.151	28.890
4	0.319	0.165	31.516
5	0.306	0.167	31.816
6	0.240	0.175	33.313
7	0.158	0.184	35.064
8	–0.019	0.202	38.574
9	–0.166	0.216	41.261
10	–0.294	0.228	43.455

to make classifications or predictions regarding the grouping of an individual data point. Usually, the smaller number of *K*, the higher accuracy should be obtained. Here *K* was varied from 1 to 10. The results are shown in Table 3. From the table, as *K* is increased, the R^2 score decreases. *RMSE* sees a similar pattern in which as *K* is increased, the *RMSE* score is getting worse. It can be understood that a higher value of *K*, makes the algorithm less sensitive to the noise. In addition, our dataset is small, and many hidden variables may exist since the mixing of PLA and plasticizer is a complex process. So, Thus, the maximum accuracy should be obtained in a low value of *K*, in our case is 1 with an R^2 score of 0.839.

3.2. SVR model performance

SVR is an ML algorithm that is built based on the Support Vector Machine (SVM) method but for regression instead of classification. Basically, SVR finds the best fit line for the data points, thus creating a hyperplane that has the maximum number of data points. The varied parameters in SVR are *C*, which is a regularization parameter to express tolerance for data point misrepresentation, and gamma, which is a parameter that determines how much curvature there is in a decision boundary. A larger gamma indicates a greater curvature at the boundary, but there is a regression problem in this case. The results of the variation of *C* and gamma are given in Table 4. From the table, it was found that the maximum R^2 score is 0.689 with a *C* and gamma of 1000 and 0.1, respectively. Considering the complexity of the relationship between features and the target, a larger tolerance is expected. However, the smaller gamma means the regression boundary curvature is not complex.

Table 4. Effect of variations in *C* and gamma values on SVR performance

C	Gamma	R^2 Score	*RMSE*	*RRMSE*
0.1	1	0.420	0.264	50.840
1	1	0.576	0.226	43.484
10	1	0.664	0.201	38.677
100	1	0.653	0.204	39.325
1000	1	0.666	0.200	38.594
0.1	0.1	0.093	0.330	63.590
1	0.1	0.464	0.254	48.874
10	0.1	0.546	0.234	44.972
100	0.1	0.671	0.199	38.295
1000	0.1	0.689	0.193	37.229
0.1	0.01	–0.086	0.361	69.558
1	0.01	0.115	0.326	62.803
10	0.01	0.448	0.258	49.620
100	0.01	0.492	0.247	47.559
1000	0.01	0.561	0.230	44.251
0.1	0.001	–0.112	0.366	70.404
1	0.001	–0.085	0.361	69.547
10	0.001	0.117	0.326	62.721
100	0.001	0.444	0.259	49.777
1000	0.001	0.480	0.250	48.122
0.1	0.0001	–0.115	0.366	70.490
1	0.0001	–0.112	0.366	70.400
10	0.0001	–0.085	0.361	69.546
100	0.0001	0.118	0.326	62.713
1000	0.0001	0.444	0.259	49.788

3.3. ANN model performance

The ANN algorithm was employed as the third model. After optimization, the following parameters were kept constant: testing set fraction to total data of 0.3, random state of 101, the activation function of ReLU for both input and hidden layers, the activation function of linear for output layer, Adam optimizer, and the mean squared error (MSE) as loss function. Here, the number of hidden layers and the number of nodes were varied to obtain the optimum R^2 score. The results are shown in Table 5. It was found that the optimum R^2 score was obtained with three hidden layers with nodes of 128, 64, and 32 for every hidden layer. Here 1000 epoch was used. Here we found that the number of layers needed is only three, although it is a common conception that the deeper the layer, the more complex the relationship could be captured. However, the number of nodes is quite large, which means the model has a wider network and the complexity of the regression boundary.

Table 5. Effect of variations in the number of hidden layers and nodes in each hidden layer on ANN performance.

Number of nodes in the layer of			R^2 score	*RMSE*	*RRMSE*
1	2	3			
8	–	–	0.507	0.153	26.860
16	–	–	0.705	0.118	20.762
32	–	–	0.560	0.144	25.377
64	–	–	0.580	0.141	24.782
128	–	–	0.690	0.121	21.279
8	8	–	0.494	0.155	27.192
16	16	–	0.641	0.130	22.920
32	32	–	0.660	0.127	22.306
64	64	–	–0.063	0.216	37.705
128	128	–	0.597	0.138	24.284
8	16	–	–0.257	0.165	29.020
8	32	–	0.424	0.165	29.020
8	64	–	0.201	0.187	32.681
8	128	–	0.684	0.118	20.567
16	32	–	0.415	0.160	27.971
16	64	–	0.160	0.192	33.515
16	128	–	0.104	0.198	34.608
32	64	–	0.082	0.201	35.040
32	128	–	0.369	0.166	29.057
64	128	–	–0.760	0.278	48.567
8	8	8	0.138	0.194	33.951
16	16	16	–0.627	0.267	46.650
32	32	32	0.525	0.144	25.195
64	64	64	–0.566	0.262	45.772
128	128	128	–0.276	0.236	41.307
32	32	8	0.529	0.144	25.108
64	64	8	0.165	0.191	33.430
64	64	32	–0.554	0.261	45.590
64	32	16	–0.143	0.224	39.104
64	32	8	–0.245	0.234	40.807
64	32	32	0.395	0.163	28.435
64	8	8	–0.674	0.271	47.325
32	8	8	–0.259	0.235	41.032
128	64	32	0.901	0.068	12.037
128	64	8	–0.171	0.227	39.584
128	32	8	0.433	0.158	27.543

This reflects the complex relationship between features and targets.

3.4. Summary of optimized model performance and performance stability

The summary of the optimized R^2 score is given in Figure 1. However, we also conduct tests on the stability of the accuracy. It was found that although ANN gives greater accuracy, the model itself has a wildly fluctuating R^2 score. This may be due to a small quantity of data since ANN needs much larger data points. Thus, we recommend KNN may be used to predict impact strength although the accuracy is smaller than ANN. The accuracy and stability of the results are shown in Figure 2.

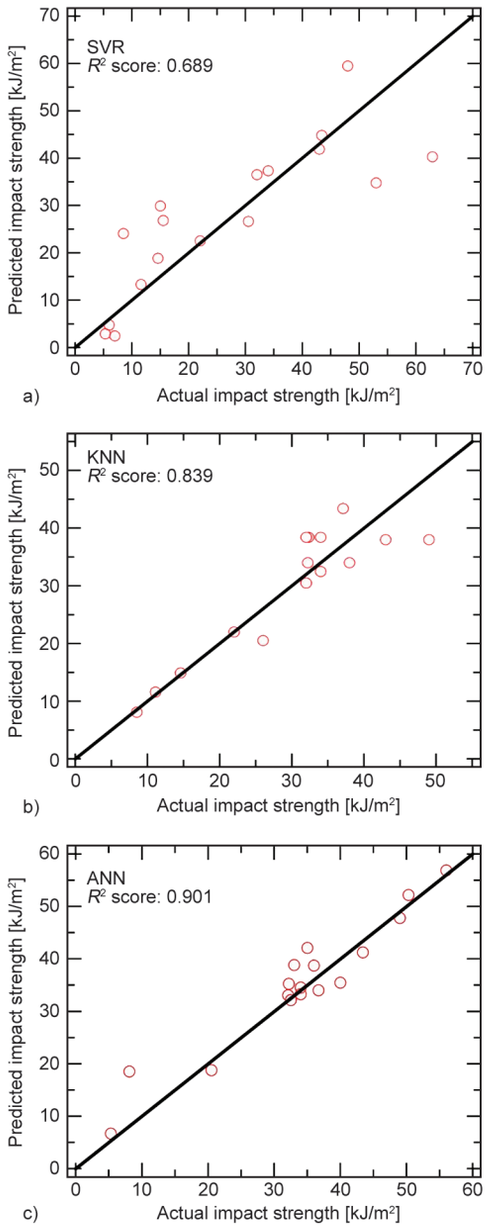

Figure 1. Optimized R^2 score plots of a) KNN model, b) SVR model, and c) ANN model.

3.5. Correlation coefficients and the feature of importance

The Pearson correlation coefficient (PCC), or correlation coefficient, measures the linear correlation between features and outputs, which is tabulated in Table 6, and the feature importance measures are presented in Table 7. It should be noted that PCC does not measure nonlinear relationships. According

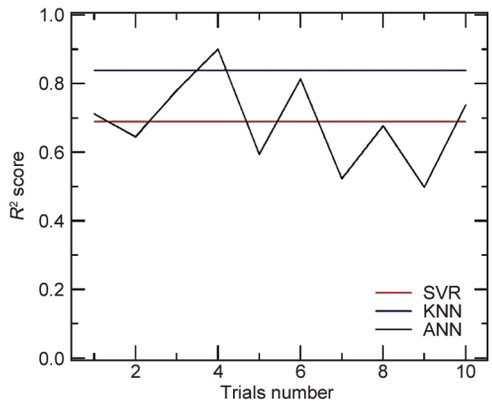

Figure 2. Performance (R^2 score) stability of KNN, SVR, and ANN models.

to Table 6, it can be seen that all of the input features are almost independent of each other. It can also be seen that plasticizer density is more correlated to impact strength in comparison to other features, followed by plasticizer molecular weight, PLA molecular weight, and plasticizer to PLA content. This means that it is preferable to change plasticizer density to observe the change in impact strength in comparison to other features. A negative sign of plasticizer density PCC means that as the plasticizer density is increased, the impact strength will likely decrease. Jacobsen and Fritz [8] conducted experiments by adding plasticizer PEG1500, glucose monoesters, and partial fatty acid esters and found that at similar plasticizer contents, the impact resistance of plasticized samples is similar, especially for glucose monoesters and partial fatty acid esters addition. The glucose monoesters and partial fatty acid esters both have similar densities of 1.06 and 1.03, respectively. As pure PLA has no plasticizer, the value of plasticizer density is zero, and according to our model, as we increase plasticizer density, the impact strength decreases, and we found that in our experimental setup, this was true, as pure PLA has higher impact strength (though Jacobsen and Fritz used impact resistance, it can be assumed that impact strength behavior will be somewhat similar). However, the

Table 7. Feature importance of ANN model.

Feature	Feature importance
PLA molecular weight	0.135
Plasticizer molecular weight	0.268
Plasticizer density	0.289
Plasticizer content	0.066

PLA-PEG1500 system cannot be explained by the model, since according to our model it should have a smaller impact strength due to the higher density of the plasticizer in comparison to glucose monoesters and partial fatty acid esters. We suggest that maybe other features affect the impact strength of the PLA-PEG1500 system, and since PCC only measures linear correlation, other effects, such as nonlinearity, could not be captured.

Similar behavior occurs for plasticizer content and PLA molecular weight, which has negative PCC. For plasticizer content, Jacobsen and Fritz [8] also reported that for glucose monoesters and partial fatty acid esters plasticizers with content above 2.5%, the impact resistance decreased as the plasticizer content was increased. Wang *et al*. [35] also reported that the impact strength of printed PLA increased with decreased molecular weight to some extent, which supports our model.

Opposite behavior was observed for the plasticizer molecular weight feature, which has a positive effect on impact strength. Jacobsen and Fritz [8] also reported that the PEG1500-PLA system has higher impact resistance than PLA glucose monoesters and PLA partial fatty acid esters, despite the fact that glucose monoesters and partial fatty acid esters have a lower molecular weight than PEG1500. The results of the feature of importance showed a similar pattern. Plasticizer density, PLA molecular weight, and PLA molecular weight have more importance on the model or prediction side, while plasticizer content does not seem to have strong importance according to the model. It can be understood that when the plasticizer content is changed, the impact strength

Table 6. Pearson correlation coefficient of plasticized PLA dataset.

	PLA molecular weight	Plasticizer molecular weight	Plasticizer density	Plasticizer content	Impact strength
PLA molecular weight	1	–0.11	0.52	0.15	–0.48
Plasticizer molecular weight	–0.11	1	–0.11	–0.31	0.50
Plasticizer density	0.52	–0.11	1	0.15	–0.58
Plasticizer content	0.15	–0.31	0.15	1	–0.04
Impact strength	–0.48	0.50	–0.58	–0.04	1

does not always increase or decrease, and the effect may be superficially random or not well understood by our model.

3.6. Experimental comparison

The experimental comparison was conducted, although the number of samples was small. The model used in this comparison is KNN. The reason is as mentioned in the discussion and results subsection that although the ANN gives more accuracy than KNN, the accuracy values are fluctuating while KNN gives stable yet reliable accuracy. The other reason for using KNN is that, based on the cross-validation that has been conducted, KNN showed a higher R^2 score than SVR and ANN.

The comparison between experiments and predictions is demonstrated in Figure 3. It can be seen that the prediction and the experimental results are close enough for the concentration of PEG1000 and OES to reach 20% concentration. It can be seen that the effect of the addition of plasticizers PEG1000 and OES is complex. Despite the limited number of experimental results, our model can predict the behavior of the impact strength. The advantage of using ML before experiments are that ML can guide experimentalists in finding the most efficient amount of plasticizer to fine-tune the target property. In our case, the experimentalist can fine-tune by varying plasticizer content to obtain maximum impact strength, which in our case study is predicted to be 4 and 5% of the concentration of PEG1000 and OES, respectively.

4. Conclusions

Three ML models, KNN, SVR and ANN to predict the impact strength of plasticized PLA have been successfully developed. It was found that ANN has the highest R^2 score of 0.901 in comparison to 0.839 of KNN and 0.689 of SVR. The optimized R^2 score of ANN was obtained at three hidden layers with 128, 64, and 32 nodes, for SVR it was optimized at C and gamma of 1000 and 0.1 respectively, and for KNN at K of 1. However, the R^2 score stability was found to be fluctuating for ANN, while KNN and SVR shows stable results. Thus, we recommend that KNN can be used as a model instead of ANN, given the small number of experimental data. This may be due to a small number of data since ANN needs much larger data points. PCC analysis revealed that plasticizer density had the highest correlation with impact strength, followed by plasticizer molecular weight, PLA molecular weight, and plasticizer content. This indicates that to some extent, it is preferable to alter plasticizer density in order to examine the effect on impact strength, as opposed to altering other characteristics. Lastly, the experimental comparison was conducted for PLA and PEG1000, and OES as plasticizers. It was found that KNN can predict the complex relationship between plasticizer content and impact strength which can not be easily captured by experiments. We suggest that our approach can be used by experimentalists to conduct the fine-tuning of optimization.

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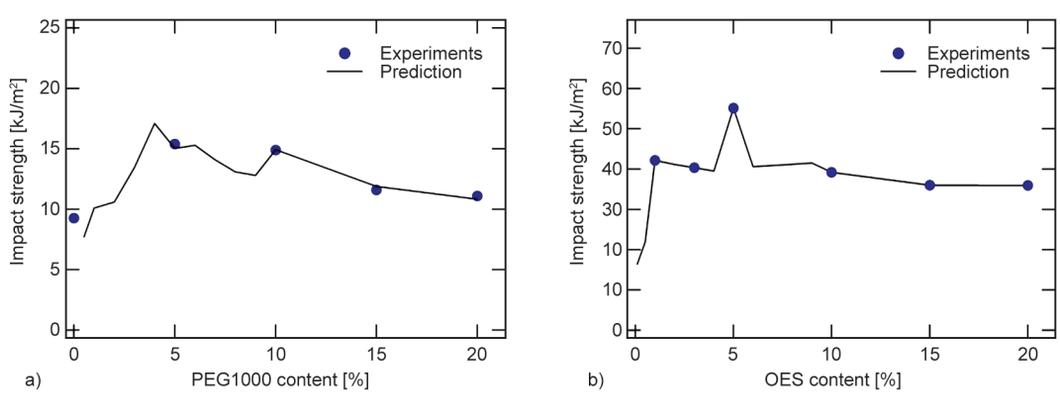

Figure 3. The impact strength prediction and the experimental results of a) PEG1000-plasticized PLA and b) OES-plasticized PLA.

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