Mechanical Property Prediction of Poly(Lactic Acid) Blends Using Deep Neural Network

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Abstract: Physical blending is one of the method to control and improve the mechanical properties of polymer such as Poly(lactic acid) or known as PLA. However, the phenomenological theory or model to connect the structure and properties of PLA blend is not available. Thus, in order to predict the mechanical property from structure is based on many trial experiments. In this study, Deep Learning Network (DNN) was employed to predict the yield strength of PLA blend based on its structure information: blending composition, molecular weight, melting point and density of polymer. It was demonstrated that DNN can successfully predict the mechanical property from structure information of PLA blends although the accuracy could be further improved.

Keywords: Polymer; Poly(lactic acid); Polymer blend; Machine Learning; Deep Neural Network

1. Introduction

Poly(lactic acid) or known as (PLA) has drawn substantial scrutiny over the last two decades due to its better properties, excellent biodegradability, and processability in comparison with other biodegradable polymers and also partly due to the increasing environmental concerns and resource crisis associated with traditional petroleum-based polymers[1,2,3,4,5]. PLA basically is a biodegradable polyester which was derived from renewable resources such as corn, sugar and potato. The good biocompatibility of PLA enables it to find huge utilizations in industrial and even in medical/bioengineering fields[6,7]. The yield strength of PLA, which is important for medical applications, is usually in the range of 30–50 MPa depending on the molecular weight and stereochemical composition. To control the yield strength (increase or decrease), one can blend PLA with various polymers available.

Besides blending, copolymerization and polymer compositing are commonly used to. However, physical polymer blending has advantages over other procedures due to easier and more cost-effective method[8,9,10]. Correspondingly, PLA blends with biodegradable and non-biodegradable polymers have been increasingly popular.

However, to predict the mechanical properties of the PLA blending is difficult due to the incompatibility. It is known that various polymers are incompatible with PLA[11,12, 13]. In addition, there is no phenomenological theory or formula to connect the physical polymer blending with mechanical properties. To better understand the correlation or connection between physical polymer blending with mechanical properties is very important to provide insights into the engineering design of polymer blending[14,15,16]. With the advancement of information technology, this problem can be alleviated with the help of artificial intelligence or machine learning methods[17]. Given the fast development of computational power and the availability of experimental data, machine learning can be used to construct prediction models of mechanical properties of PLA blend.

Various machine learning available, and one of most commonly used is Neural Network (NN). NN is a machine learning technique which mimics the structure of the brain and largely human nervous system. NN consists of three main processing units: input, hidden and output layers. NN is so popular that it is used in a variety of problems including classification, regression, pattern recognition, dimensionality reduction, computer vision, and predictive analysis.

Deep Neural Network (DNN) is a type of NN modeled as a multilayer perceptron (MLP). MLP is algorithms trained to learn various representations from sets of data without a design of feature extractors. DNN is popularly called Deep Learning (DL). DNN consists of a higher or deeper number of processing layers. DNN also allows for

more complex and non-linear functions to be modeled. DN improvement has been complemented by the abundance of cheaper processing units and the availability of big data to train from, in which in materials engineering case the availability of shared experimental data.

In this paper, we investigated the use of DNN to predict mechanical property (yield strength) of PLA blends based of structure (blend composition, molecular weight, melting temperature etc.). So far, there is no dedicated paper to discuss this issue. Our goal is to pioneer the use of DN to have better understanding the correlation between structure and properties of PLA blends.

2. Data and Methods

2.1 Data Collection and Feature Selections

The experimental data was obtained from a database provided by the Japan National Institute of Material Science (NIMS). This database contains the world's largest experimental datasets. There is one dedicated NIMS part to polymer: Polymer database (Polyinfo). Polyinfo database contains blend composition, weight formula, density and melting point as well as various mechanical properties such as tensile at yield (yield strength), tensile at break, impact etc. Yield strength is defined as maximum stress that can be handled by material without undergoes plastic deformation.

There are 60 datasets of PLA blends, but there are 20 in complete datasets. Total, there are 40 datasets which are used in this study. The input of our DNN algorithm are composition (blending composition), molecular weight, melting point and density of polymer which will be blended to PLA. Composition, molecular weight, melting point and density is related to the thermodynamics of physical polymer blending. The output of our DNN algorithm is the yield strength of polymer. The features information is given in table 1 while the output of the data (yield strength/MPa) has min of 12, max of 81.4, mean of 52.69 and standard deviation of 14.10.

Table 1. Features of 40 the NIMS yield strength data

No	Features	Min	Max	Mean	Std. Dev.
1.	Non PLA composition (%)	1	60	18.40	14.88
2.	Non PLA weight formula	51	254.8	126.22	58.78
3.	Non PLA density (gram/cm^3)	0.9	1.42	1.06	0.14
4.	Melting Temperature (K)	271.15	633.15	430.94	120.64

2.2 Data Pre-Processing

Data pre-processing steps will be performed using feature scaling. Feature scaling is an important stage of the preprocessing stage that determines how good the data transformation is. This will lead to good data that is on a uniform scale with value range within 0 to 1[18]. This data pre-processing is called by using the following command:

```
scaler_x = MinMaxScaler().fit_transform(X)
scaled_y = MinMaxScaler().fit_transform(y.resha
pe(len(y),1))[:,0]
X = StandardScaler().fit_transform(scaler_x)
y = StandardScaler().fit_transform(y.reshape(le
n(y),1))[:,0]
```

After pre-processing, the dataset will be split into training and testing dataset with the ratio of 80% training dataset 20% testing dataset, and random state is 8. This splitting data is called by using the following command:

```
X_train, X_test, y_train, y_test = train_test_s
plit(X, y, test_size=0.2, random_state=8)
```

3. Results and Discussion

The process of creating DNN algorithms use the help of Google Colab, which is a coding environment with the python programming language to create algorithms and perform data processing. In this research the outputs are produced in the form of values from yield strength from DNN model architecture with the help of activation function, layer and dense on a model network which are designed by utilizing the tensor flow library. Activation function use in this research is ReLU used in each hidden layer which is used to process the input by updating the weight that produces the output. In addition to the activation function in modeling, the optimizer is also determined. Optimizer is used to gain good performance on the model.

This research utilizing the “Adam” optimizer that is advantageous on eliminating the gaps in data generalization[19, 20]. This allows for more precise control of the direction and rare size to be able to update the weight vector so as to minimize the loss function and increased model performance[21]. In making the algorithm, several other parameters are also needed that can help the model training process. One of these parameters is epoch, which is a parameter that determines how many times the algorithm learns and works on the entire training dataset with the aim of correcting any error[22]. Another one is batch size, which is a parameter used to determine the number of data samples that work before the model parameters are updated[23].

The purpose of this paper is to provide mechanical property prediction of poly-(lactic acid) blends using deep learning and regression models. Prediction was made using these models and estimations score method using R^2score to evaluate the model as a regression metrics. This metric is an estimated tested target variable or y_test with predicted value as a target provided by the model. R^2score provides information about how close the prediction of the model is to the target variable and is used specifically in regression analysis.

The performance of the machine learning regression model using Deep Neural Network or Deep Learning is measured by correlation coefficient (R^2). R^2 score evaluates predictive performance of DN algorithm as a

regression score function to correlate between true and predicted value using proportion of variance. The highest R^2score is 1.0, and can be negative if the model's prediction is bad or really far from the true value. A constant model that always predicts the expected value of y, regardless of input characteristics, receives a score of 0.0[24, 25]. The results are given in **Fig 1** for training and testing data scatter plot for DNN regression.

Fig 1. shows the scatter plot for the regression model to Poly(lactic acid) blends using DNN with R^2score of 0.953 from two sets : 20% data for testing and 80% of the training dataset, calculated from below[25] :

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

where n is the number of testing data, and y is actual value,$\hat{y}$ is the predicted value and $\underline{y}$the average value[25].

From the plots in **Fig. 1**, DNN extracted from the best fit on test data with parameters of batch size is 64, two hidden layers with dense 32 and 16, and epoch is 1000. R^2score of 0.953 indicated the representation between normalized measured yield strength and normalized measured predicted yield strength using the testing dataset using independent variables previously defined and also shows a strong correlation between normalized measured yield strength and normalized measured predicted yield strength values with high R^2score. This result demonstrates that DNN can successfully predict mechanical property from structure information of PLA blends although the accuracy can still be improved.

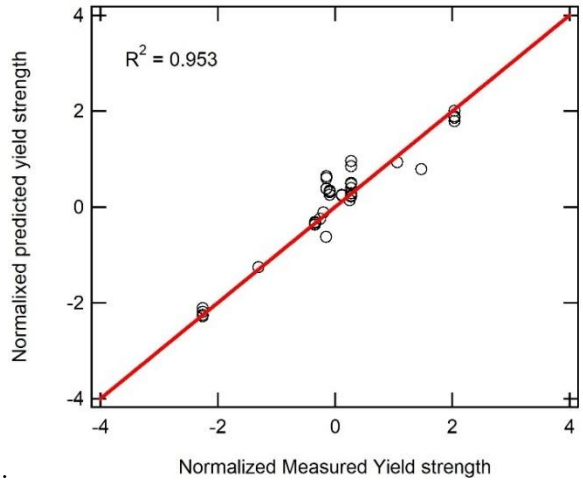

Fig. 1: Scatter Plot for Regression Model to Poly(lactic acid) blends using Deep Learning

4. Conclusion

We have successfully demonstrated the use of DNN as prediction tool for mechanical property of PLA blends. The accuracy which is represented by R^2score is 0.953. Our result demonstrates that DNN can succesfully predict mechanical property from structure information of PLA blends although the accuracy can still be improved.

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