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Investigating Features and Output Correlation Coefficient of Natural Fiber-Reinforced Poly(lactic acid) Biocomposites

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Abstract. Polylactic acid (PLA) material has the potential to be applied in various industrial fields, but this material has shortcomings in terms of mechanical properties, especially mechanical strength, due to brittleness nature of PLA. The manufacture of PLA composite material with the addition of natural fibers as a reinforcing phase is one of the methods to increase the impact strength and maintain the biodegradable properties of the material. However, in theory, there are many factors that affect the mechanical properties of composite materials, thus making the mechanical properties of composites more complex than monolithic materials. The mechanical properties of these composite materials can be predicted using deep learning by paying attention to the relationship between factors, and between factors and their mechanical properties. This relationship has an important role in creating a predictive model with good accuracy. Therefore, correlation analysis is an important thing to do. Correlation analysis was applied using Python programming language to determine the relationship between the impact strength of natural fiber-reinforced PLA biocomposites with its feature information: chemical composition, density, dimensions, surface chemical treatment of natural fibers, matrix-reinforcement volume fraction, and the type of processing used to manufacture the material.
Keywords: PLA; composite; Natural fiber; deep learning; biodegradable.

INTRODUCTION

Material is something that has been integrated with all lines of life, where almost every activity involves the use of materials (Hopewell *et al*., 2009). Therefore, research in materials science continues to develop along with technological developments. Looking at the current environmental conditions, environmental damage becomes a major issue every year, one of which is due to the large number of non-environmental-friendly materials that cannot be degraded naturally. Therefore, in this era, research in materials science does not only focus on the mechanical properties of materials but also considers the effects that materials will have on the environment (Kumar *et al*., 2003).

According to this situation, the polymer is one of the materials that can overcome this problem. Besides its advantages, several types of polymer materials can be degraded naturally and are environmentally friendly. This type of polymer is a polymer that comes from nature, such as animals or plants. The natural polymer material that is currently a concern in the research of environmentally friendly materials is polylactic acid (PLA) (Fatriansyah *et al*., 2022; and Rahmat *et al*., 2020). PLA is a natural polymer material that has the potential to be applied in various applications because of its unique and superior mechanical properties. PLA has a relatively high tensile strength, is light, biodegradable, biocompatible, and has good processing ability, where PLA can be processed using standard plastic manufacture in general (Rashdan *et al*., 2016). Besides these advantages, PLA has poor toughness and impact strength (Rasal *et al*., 2010). Therefore, it is necessary to modify PLA to overcome these shortcomings by making PLA into a composite material by mixing other materials as reinforcement (Fatriansyah *et al.*, 2022). To maintain the environmentally friendly or biodegradable properties of PLA composite materials, support is used, which can also be naturally degraded.

This PLA biocomposite material has the potential to be applied in various fields of application, where each application demands different specifications of mechanical properties. Deep learning is one of the technologies that can predict biocomposites' mechanical properties based on factors that affect them (Rahman *et al*., 2021; Fathi *et al*., 2020; and Rong *et al*., 2019).

But, building a deep learning predictive model from many factors or features that affect the output will be challenging (Arunika *et al*., 2022). Therefore, it is necessary to know the factors that influence its mechanical properties and how they affect the mechanical properties to produce biocomposite materials with the desired mechanical properties from an excellent accurate deep learning model. This relationship can be determined traditionally through testing the composite materials by varying the materials and processing parameters, but this is difficult to do and will take a long time; moreover, many factors affect the mechanical properties of biocomposites (Senthil Muthu Kumar *et al*., 2020; and Muthuraj *et al*., 2016). These relationships are non-linear, so the process becomes ineffective. Correlation analysis using Python programming language is an effective and fast method to know how features correlate with each other, how features correlate with the output, and how strong the correlation is. With this method, it will be easier for us to make feature selection and determine the most valuable features, resulting in good model performance.

DATA AND METHODS

Data used for this research are secondary data collected from previous research about the influence of natural fiber chemical composition, density, dimension, and chemical surface modification, as well as PLA matrix-natural fiber reinforcement volume fraction and PLA biocomposites manufacturing method. Information collected for this research are: cellulose, hemicellulose, lignin, pectin, wax, and moisture content of the natural fiber, fiber density, fiber diameter, fiber surface modification (treated or untreated), fiber content in composites, composites manufacturing method (injection or compression molding), as well as mechanical properties of the, resulted from PLA composites such as impact strength. Impact strength is defined as the resistance of a material to fracture by a blow, expressed in terms of the amount of energy absorbed by the material before fracture.

Twenty-seven data used in this study have been collected based on the above information. Before the deep learning modeling stage, these features and output would be applied to correlation analysis to get the most suitable features as the input. The statistical information of the features is given in TABLE 1. At the same time, the output of the data, which is impact strength, has a minimum value of 5.00 KJ/m^2, a maximum value of 56.00 KJ/m^2, and a mean of 19.86 KJ/m^2, and a standard deviation of 11.97 KJ/m^2.

TABLE 1. Features statistical information of 27 data points

Features	Min	Max	Mean	Std Dev
Fiber Cellulose (%)	34.50	89.00	64.98	14.07
Fiber Hemicellulose (%)	4.00	21.00	16.05	5.19
Fiber Lignin (%)	0.75	26.00	8.38	8.69
Fiber Pectin (%)	0.20	6.00	1.97	1.59
Fiber Wax (%)	0.00	0.60	0.10	0.22

Features	Min	Max	Mean	Std Dev
Fiber Moisture (%)	0.00	12.60	7.10	4.89
Fiber Treatment	-	-	-	-
Fiber Content (%)	5.00	40.00	25.00	11.09
Fiber Diameter (μm)	10.50	179.0	52.09	53.79
Fiber Density (g/cm^3)	1.13	1.56	1.41	14.00
Processing Method	-	-	-	-

RESULTS AND DISCUSSIONS

The correlation analysis process uses the help of Google Colab, which is a coding environment with Python as the programming language to perform various data manipulation, analysis, and visualization. Before analyzing the data, data reading, cleaning, and exploratory data analysis were conducted first using the panda's library to produce clean data and to know the characteristics of the data.

After getting clean data and doing exploratory data analysis, correlation analysis was then conducted to know how strong the correlations are between each feature, as well as between features and the output. The correlation coefficient will describe whether a feature is highly related or not with other features or to the output. The magnitude of the correlation coefficient is expressed through the following equation :

$$r_{(x,y)} = \frac{COV_{(x,y)}}{s_x s_y} \tag{1}$$

$$COV_{(x,y)} = \frac{\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y})}{n-1} \tag{2}$$

where $COV_{(x,y)}$ is the covariance of the variables x and y, n is a number of data points, $\bar{x}$ is mean of the variable x, $\bar{y}$ is mean of the variable y, $r_{(x,y)}$ is the correlation of the variables x and y, s_x is the standard deviation of the variable x, and s_y is the standard deviation of the variable y. (Sands, 1977)

Based on the equation above, the resulting correlation coefficient has a value that falls in the range of -1 to 1. If the correlation coefficient is 1, the variables have a perfect positive correlation, which means that the variables move proportionally in the same direction. If the correlation coefficient is 0, it means that there is no relationship exist between the variables. On the other hand, if the correlation coefficient is -1, the variables have a perfect negative correlation (inversely correlated), which means if one variable increases, the other variable decreases proportionally. (Schober *et al.,* 2018)

The correlation analysis conducted between each feature is shown in FIGURE 1. There are some features that are highly correlated with each other, such as cellulose and hemicellulose, as well as cellulose and lignin. In order to get a good deep learning regression model performance, one of the highly correlated features must be removed.

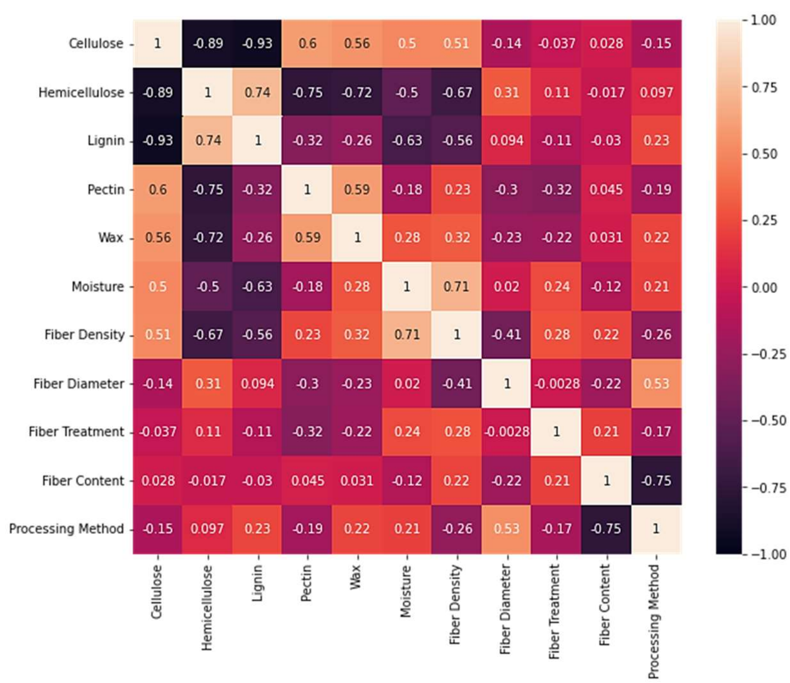

FIGURE 1. Correlation coefficient between each feature

The correlation between features and the output (impact strength) is shown in FIGURE 2. Based on the plot, there are some features that have a correlation coefficient of almost zero. They are processing method with correlation coefficient of -0.066, fiber surface chemical treatment with correlation coefficient of 0.055, cellulose with correlation coefficient of 0.086, and fiber density with correlation coefficient of 0.098. It means that there is almost no relationship between those features and the output.

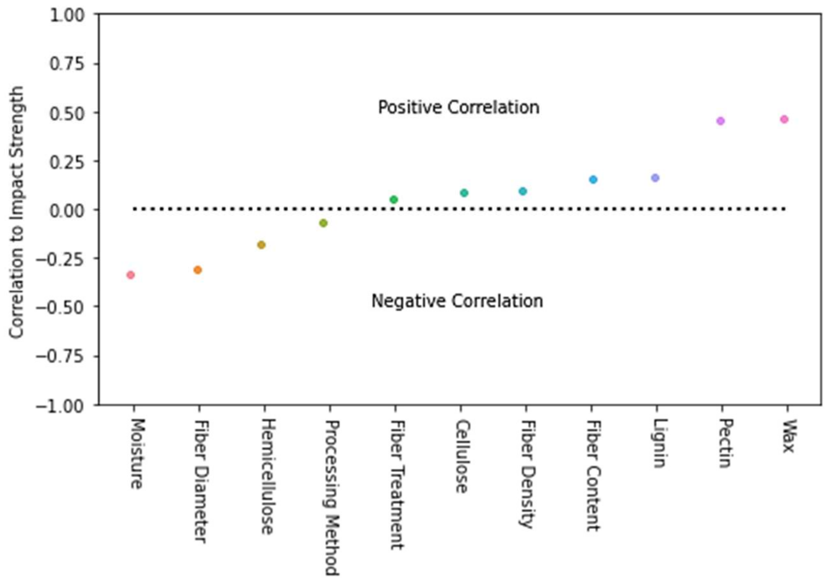

FIGURE 2. Correlation coefficient between features and the output

CONCLUSION

Based on correlation analysis that have been conducted, it shows that cellulose has high correlation with hemicellulose and lignin, as well as has low correlation with impact strength as the output. Therefore, cellulose has to be removed to increase deep learning model performance. This also applies to other features such as processing method, fiber surface chemical treatment, and fiber density, as they also have low correlation coefficient with impact strength as the output. Thus, there are 7 features that been used in this research to make a good deep learning model performance which are: hemicellulose, lignin, pectin, wax, and moisture content, as well as fiber diameter and fiber content.

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