

Performance Study of Intercalated Meltblown Nonwoven Materials Based on Gaussian Process Regression

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Abstract: The demand for face masks is on the rise due to the COVID-19 pandemic. Melt-blown nonwoven material is an important raw material for mask production, and its structural variables determine the performance of the final product. In this paper, the prediction model between structural variables and product performance is established, and the relationship between structural variables and product performance is obtained by using Gaussian process regression method, and the prediction model is tested to further verify the reliability of the model. The experimental results show that. The prediction accuracy of the model based on Gaussian process regression is high, and the average absolute error is less than 0.2, so the prediction method is effective. The final experimental results have a certain degree of reference significance for the study of the influence of the structure variables of intercalated melt-blown nonwovens on the product properties, which is helpful to provide a certain theoretical basis for the establishment of the control mechanism of product properties.

Keywords: Structure variables; Properties of products; Gaussian process regression; Intercalated melt-blown nonwoven material

1. Introduction

Due to the occurrence and rapid spread of the "New Coronavirus Outbreak", masks are becoming a daily necessity for People's daily travel. In the country, people use up to 530 million masks daily and the use of masks continues to increase. The New Coronavirus Outbreak has led to a number of projects in the materials industry, such as the protective clothing industry and the medical alcohol industry.

As masks are gradually being integrated into people's lives, public demand for their quality and protective capacity is also increasing. N95 masks, medical surgical masks and single-use medical masks that meet national standards have a protective function and meet the requirements of epidemic prevention, so the use of raw materials for masks is crucial.

Meltblown non-woven material [1] is an important raw material for the production of masks and has received widespread attention from domestic and international companies because of its excellent filtration properties, its simple production process, low cost and light weight, which make it outstanding in terms of filtration, bacterial barrier and adsorption. However, due to the very fine fibres of meltblown nonwoven materials, their performance is often not guaranteed during use due to poor compression resilience [2]. As a result, scientists have created the intercalation meltblown method, in which fibres such as polyester (PET) staple fibres are inserted into the meltblown fibre stream during the meltblown preparation of polypropylene (PP) to create a 'Z-shaped' structure of the intercalated meltblown non-woven material. It is a method of forming a web of microfibrils. Meltblown nonwovens are made up of ultra-fine fibres with a diameter of less than 4 μm. The resulting nonwoven has a soft feel and good filterability.

There are more parameters for the preparation of intercalated meltblown nonwoven materials [3], and there are also interactions between the parameters, plus more complex after the intercalation airflow. Therefore, the study of the final product performance determined by structural variables, which are determined by process parameters, also becomes more complex. By establishing the relationship model between structural variables and product performance, it helps to provide some theoretical basis for the establishment of product performance regulation mechanism.

2. Gaussian process regression

Gaussian Process Regression (GPR) was proposed as a general approach to machine learning by Carl E. Rasmussen, a scholar at the University of Cambridge, and Christopher K. I. Williams, a scholar at the University of Edinburgh. Their study published in 1996 gives the solution system of GPR by function space view and discusses the maximum likelihood estimation of GPR hyperparameters [4] and Monte Carlo methods [5] to solve. Gaussian process regression [6] is a nonparametric model for regression analysis of data using a Gaussian process prior. Its model assumptions include both regression residuals [7] and Gaussian process prior, and the solution process is performed as a Bayesian inference. In addition, GPR can provide a posterior for the prediction results and the posterior has an analytic form when the likelihood is normally distributed [8].

Thus, GPR is a probabilistic model with generalizability and resolvability [9]. Based on the convenient properties of Gaussian processes and their kernel functions, GPR has been applied to problems in the fields of time series analysis [10], image processing [11] and automatic control [12]. GPR is a computationally expensive algorithm and is usually used for regression problems with low and small samples, but it also has extended algorithms for large samples and high-dimensional cases.

The solution of GPR, also known as superparametric learning, is the process of determining the unknowns in the kernel function [13] by learning samples according to the Bayesian approach [14]. Gaussian process regression is a parametric-free kernel method in a Bayesian learning framework. It generates a nonparametric model [15] by directly modeling the function. The regression equation for the training input data $X = x_1, x_2, x_3, \dots, x_n, x^*$ and its corresponding output data $Y = y_1, y_2, y_3, \dots, y_n, y^*$ is where:

$$Y = f(x) + N(0, \sigma_n^2), f(x) \sim G(0, K) \quad (1)$$

The regression function $f(X)$ does not need to be specified in a specific form and can be considered as an infinite dimensional point obtained by sampling in the Gaussian regression process; $N(0, \sigma_n^2)$ denotes noise with mean 0 and variance σ_n^2 .

$G(0, K)$ is a Gaussian regression process with a mean of 0 and covariance of K ; For the new input x^* and with the corresponding output y^* still have the same mapping relationship.

Using the covariance function, i.e., the kernel function to reflect the interrelationship between data points in the Gaussian regression process, the radial basis [16] (RBF) kernel function is selected as the covariance function in this topic.

$$K(x, x') = \sigma_f^2 \exp\left[-\frac{(x-x')^2}{2l^2}\right] \quad (2)$$

In the function, $K(x, x')$ is the covariance between x and x' , and l is an adjustable parameter.

Asking to take a new input x^* and its corresponding output y^* still satisfying the above Gaussian distribution, equations (3) and (4) can be derived using the above covariance matrix.

$$\begin{bmatrix} y \\ y^* \end{bmatrix} \sim N\left\{0, \begin{bmatrix} K & K_*^T \\ K_* & K_{**} \end{bmatrix}\right\} \quad (3)$$

$$\begin{cases} K = K(x, x) \\ K = K(x, x^*) \\ K_*^T = K(x^*, x) \\ K_{**} = K(x^*, x^*) \end{cases} \quad (4)$$

According to the Bayesian regression method, the conditional distribution of the predicted data y^* , $P(y^* | y)$, obeys the following Gaussian distribution.

$$y^* | y \sim N(K_* K^{-1} y, K_{**} - K_* K^{-1} K_*^T) \quad (5)$$

The mean value of the distribution can be used as an estimate of y^* .

$$y' = \text{avg}(y^*) = K_* K^{-1} y, K_{**} \tag{6}$$

The covariance of the distribution indicates the uncertainty of the predicted value.

$$k_{y'} = K_* K^{-1} K_*^T \tag{7}$$

Thus, the Gaussian process regression model can not only simulate any black box model[17], but also calculate confidence intervals, i.e., calculate the uncertainty of the simulation.

3. Experimental analysis

3.1 Build predictive models

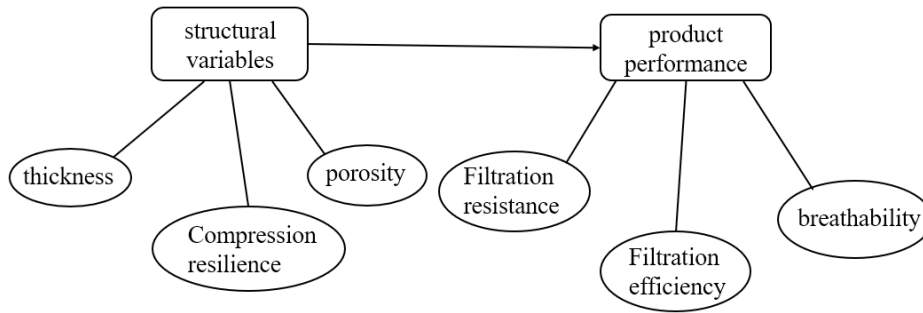


Figure 1: Relationship between structural variables and product performance

In order to investigate the relationship between structural variables and product performance of intercalated meltblown nonwoven materials, the structural variables and product performance are shown in Figure 1. A Gaussian process regression prediction model was established with thickness, porosity, and compression resilience as independent variables, and filter resistance, filter efficiency, and permeability as dependent variables, respectively. The data set samples in this paper are shown in Table 1, where the data sets are randomly sampled with 7:3 as the training set and test set, respectively. First, according to the model assumptions, there are:

Table 1: Structural variables and product performance data set

Number	Thickness (mm)	Porosity (%)	Compression resilience (%)	Filtration resistance (Pa)	Filtration efficiency (%)	permeability (mm/s)
1	1.775	94.120	88.760	17.800	30.967	455.700
2	1.891	94.155	87.621	40.256	53.212	415.756
3	2.910	96.410	86.650	7.200	24.967	968.630
4	2.183	94.655	86.938	33.230	73.042	407.455
5	3.160	96.463	85.591	19.676	40.508	530.758
6	2.235	95.030	86.040	19.230	20.767	347.230
...						
124	3.061	96.290	86.889	24.110	43.357	490.599
125	2.515	96.372	87.223	30.809	49.623	432.978

$$G(x) = g(x) + \varepsilon(x) \tag{8}$$

Here $g(x)$ is the true value of the data and $\varepsilon(x)$ obeys a normally distributed random noise sequence with mean 0 and variance σ^2 . Under the assumption that $g(x)$ satisfies a Gaussian process.

$$g(x) \sim GP(m(x), Kg) \tag{9}$$

Here $m(x) = E[g(x)]$ is the mean and Kg is the covariance matrix, also known as the kernel function. The data are processed so that the mean is zero and the kernel function is chosen as follows:

$$k_g(x_i, x_j) = c_0 \exp(-(x_i - x_j)^2 / 2\sigma_0^2), K_g = (k_g(x_i, x_j))_{n \times n} \tag{10}$$

The hyperparameters $\theta = (c_0, \sigma_0, \sigma)$ are determined by great likelihood estimation with a prior likelihood function of the negative logarithm of the conditional probabilities of the training set:

$$L(\theta) = -\log(P(y|X, \theta)) = \frac{1}{2} C^{-1} y + 12|C| + \frac{n}{2} \log 2\pi \tag{11}$$

Fixing X and finding the hyperparameter θ so that L(θ) is maximized, the partial derivative of the hyperparameter yields:

$$\frac{\partial L(\theta)}{\partial \theta_i} = \frac{1}{2} \text{tr}((\alpha\alpha^T - C^{-1}) \frac{\partial c}{\partial \theta_i}) \tag{12}$$

Of which, $C = K_n + \theta^2 I, \alpha = (K_n + \theta^2 I)^{-1} y$

3.2 Model solutions

The conjugate gradient method [18] is used to allow the partial derivatives to be minimised so as to obtain the optimal solution for the hyperparameters[19]. Once the hyperparameters are obtained, the relationship between the structural variables and the product performance can be obtained and this is used to make predictions and solve for G(x), yielding the relationship between the structural variables and the individual product performance.

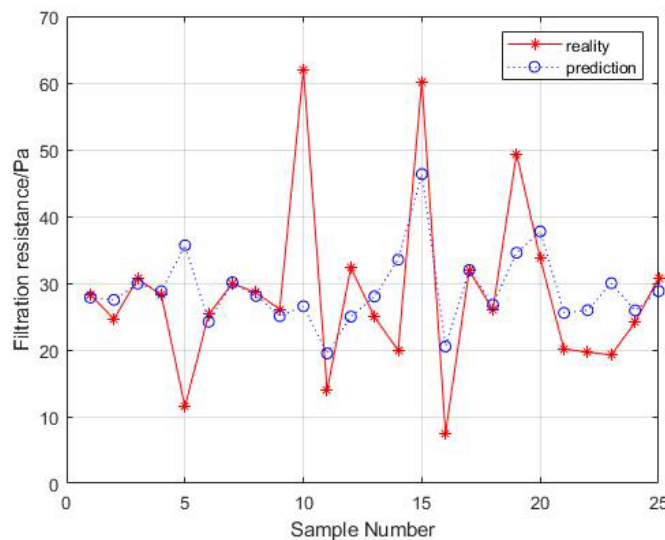


Figure 2: GPR prediction of filtration resistance results

Taking the filtration resistance as an example, the prediction results for the structural variables and filtration resistance of the intercalated meltblown nonwoven material were calculated and solved as shown in Figure 2, which shows that the Gaussian process regression has better prediction results.

3.3 Analysis of results

Using the same training data and test data in Table 1, a BP neural network[20] prediction model was constructed as a comparison test, as shown in Figure 3. To improve the predictive power of the BP neural network model, min-max normalisation was applied to the training and test data. Through several experiments, the 3-8-1 network structure was optimally selected, i.e. the network has 3 layers, the input layer contains 3 nodes, the hidden layer contains 8 nodes, the output layer contains 1 node and

the learning rate is set to 0.2.

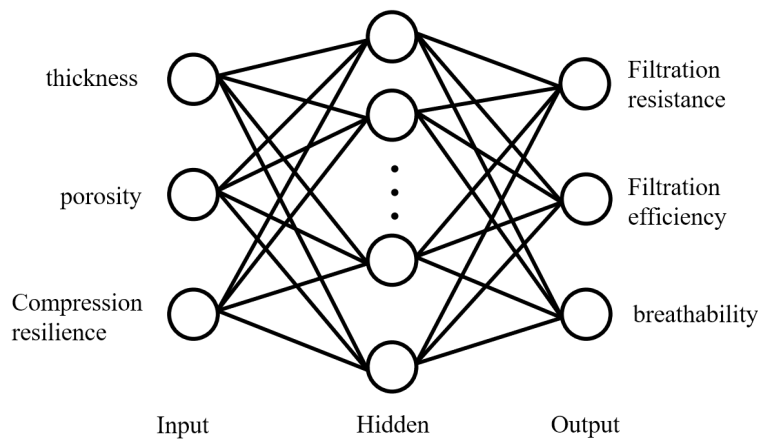


Figure 3: Neural network structure

Again using the example of filtration resistance, the calculation was solved to produce the predicted results for the structural variables and filtration resistance of the interleaved meltblown nonwoven material as shown in Figure 4.

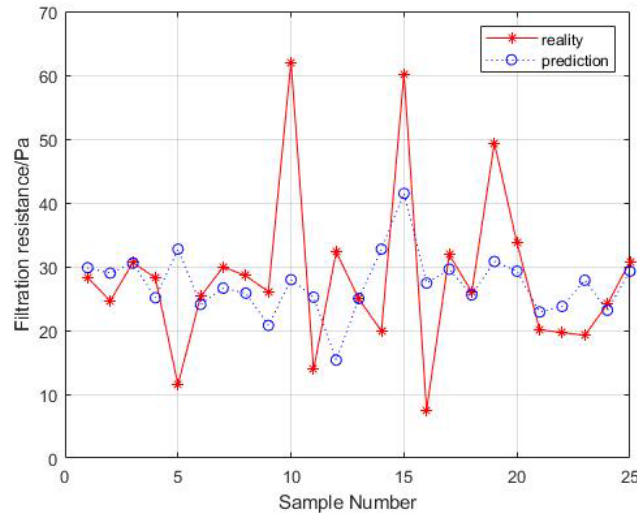


Figure 4: BP neural network prediction of filtration resistance results

From Figure 4, it can be seen that the prediction model constructed by using BP neural network has certain prediction effect in predicting structural variables and filtering resistance. In order to compare the prediction accuracy of Gaussian regression prediction model and BP neural network prediction model, for the established prediction model, this paper uses MAE experimental value, RMSE experimental value and R² as the model prediction result evaluation indexes, and compares the prediction accuracy of the constructed Gaussian regression prediction model with The prediction accuracy of the constructed Gaussian regression prediction model and the BP neural network model are compared and analyzed, and the results are shown in the following table.

Table 2: Model evaluation indicators

Product performance	MAE		RMSE		R ²	
	BP Neural network	GPR	BP Neural network	GPR	BP Neural network	GPR
Filtration resistance	0.923	0.160	8.230	5.188	0.733	0.860
Filtration efficiency	0.704	0.184	12.608	6.110	0.750	0.930
permeability	10.8633	0.096	145.378	54.558	0.830	0.886

As shown in Table 2, the values of the relevant indexes of the prediction model can be calculated based on the prediction results, and the experimental values of MAE of the Gaussian process regression model are all lower than 0.2, indicating that the average absolute error is small; the experimental value of RMSE accounts for about 10% of the original data, indicating that the error between the predicted value and the original data value is about 10%, and the error value is small; R2 is all greater than 0.86, which is better than the BP neural network model, and is closer to 1 close to the original data, indicating that the predicted data fit better with the original data.

4. Conclusion

Application of a Gaussian process regression prediction model to the study of the properties of interleaved meltblown nonwoven materials. Construct a relationship between structural variables and product performance, using thickness, porosity and compression resilience as independent variables and filter resistance, filtration efficiency and permeability as dependent variables to establish a Gaussian process regression prediction model. The conjugate gradient method is used to allow the partial derivatives to be minimized, resulting in an optimal solution for the hyperparameters. The relationship between structural variables and product performance can then be obtained and predictions can be made accordingly, yielding predicted results. A BP neural network prediction model was constructed as a comparison experiment and the analysis of the two sets of experimental results shows that Gaussian process regression is effective for the study of the properties of intercalated meltblown nonwoven materials and the prediction results are more accurate compared to the BP neural network. Gaussian process regression is superior when dealing with small samples of experimental data and can provide a more effective solution. The experimental findings show that the Gaussian process regression prediction method can be used as a theoretical basis for the control of process parameters and is of guidance.

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