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CONSTRUCTION METHOD OF GENERALIZED REGRESSION NEURAL NETWORK SURROGATE MODEL BASED ON KRIGING FITTING DEVIATION

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ABSTRACT

In the process of simulation optimization of complex electromechanical products, the complexity model is usually reduced by constructing a surrogate model. The generalized regression neural network (GRNN) surrogate model is one of the most frequently used methods in the process of establishing a surrogate model. GRNN has strong nonlinear mapping ability and flexible network structure, as well as a high degree of fault tolerance and robustness, so it is suitable for solving nonlinear problems. but the fluctuation deviation in the construction process seriously affects the accuracy of the surrogate model. Aiming at the fluctuation deviation generated in the construction of GRNN neural network, a method of constructing Generalized regression neural network surrogate model based on Kriging fitting deviation is proposed. The method first calculates the fluctuation deviation value of the Generalized regression neural network surrogate model, and the fluctuation deviation value is approximated into a multivariate normal distribution form. Then the multivariate normal distribution deviation is fitted in Kriging, Finally the corresponding value of the multivariate normal distribution deviation is subtracted from the Generalized regression neural network surrogate model. Experimental results show that this method can effectively reduce the fluctuation deviation and improve the accuracy of the Generalized regression neural network surrogate model.

Keywords: Generalized regression neural network, fluctuation deviation, surrogate model, Kriging interpolation

1. INTRODUCTION

For complex electromechanical products, it is necessary to improve the design efficiency continuously. Meanwhile it should ensure the quality of the products. Product quality requires the optimization of product performance constantly. The process of product performance optimization is an expensive simulation optimization process involving multiple disciplines [1]. Although the computing performance of computers had been improved greatly, the complexity of analytical calculations in engineering is increasing constantly.

The surrogate model replaces the computationally intensive complex simulation model with some mathematically simple analytical models. The surrogate model can reduce the computational complexity greatly and shorten the product development cycle. The surrogate model needs some experimental data at the first in the project, then uses the experimental data and selects the appropriate surrogate model to construct the interrelationships contained in the project, and then uses the surrogate model to predict in the project.

There are many surrogate models on the current. These surrogate models are being refined constantly. The most popular surrogate models are polynomial response surface method, Kriging interpolation [2], Gradient enhanced Kriging (GEK) [3], Radial basis function method (RBF) [4]，[5], Support Vector Regression Method (SVR), Artificial Neural Network (ANN) [6], and Generalized Regression Neural Network (GRNN).

Generalized Regression Neural Network (GRNN) was put forward by American scholar Specht in 1991 [7], which is a kind of radial basis neural network. GRNN has the strong nonlinear mapping ability and flexible network structure, also it has the high fault tolerance and robustness, it is suitable for solving the nonlinear problems. GRNN has a stronger advantage than RBF network in approximating ability and learning speed. Finally, the network converges on the optimal regression surface with more sample size accumulation. Meanwhile, the prediction effect is better when the sample data is less [8]. In addition, the network can handle the unstable data. Therefore, GRNN has been used in various fields widely such as signal processing, structural analysis, education, energy, food, medicine, finance, and biology. Related to this article, Nobuo NAMURA, Koji

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SHIMOYAMA et al. [9] and Jun Zheng, Xinyu Shao, Liang Gao et al. [10] proposed Kriging and RBF mixed response surface methods for highly nonlinear functions, which RBF neural network is approximated low-frequency terms and Kriging interpolation is approximated high-frequency term. Kriging interpolation is used the cross-validation method to fit the high-frequency characteristics of the function, but which can require a lot of computation time. In order to reduce the calculation time, it is necessary to reduce the amount of data used in this part, which will lead to the final accuracy of the compositing function is not high enough. This article mainly deals the variation of the generalized regression neural network in the fitting, and uses Kriging interpolation to fit this fluctuation error.

Aiming at the fluctuation of the prediction accuracy of the generalized regressive neural network when dealing with complex problems [11], this article constructs a generalized regression neural network surrogate model construction method based on the Kriging interpolation fitting deviation (Kriging-GRNN,KGRNN).This method through the different training sets, the fluctuation deviation generated by the generalized regression neural network in the fitting is extracted, and the fluctuation deviation is approximated as a multivariate normal distribution. Then, the Kriging interpolation is used to fit the multivariate normal distribution function in the fitting interval, and the multivariate normal distribution solved by Kriging interpolation is subtracted from the trained generalized regression neural network. Finally, the method is validated by using different test functions and engineering examples.

2. GENERALIZED REGRESSION NEURAL NETWORK AND KRIGING INTERPOLATION ALGORITHM DESCRIPTION

2.1 The working principle of GRNN

Generalized Regression Neural Network is a four-layer neural network, including input layer, pattern recognition layer (radial-based neurons), linear summation layer and output layer. As shown in FIGURE 1.

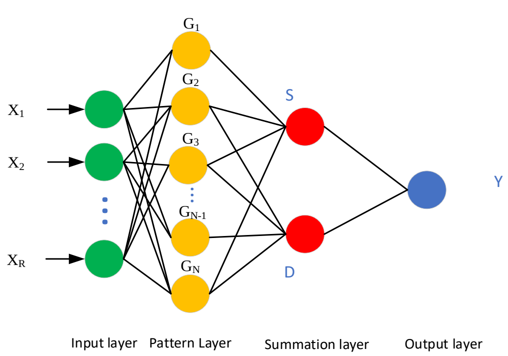

FIGURE 1: Structure of generalized regression neural network

the number of processing units in the input layer R is equal to the number of components of the input vector, the number N of neurons in the intermediate pattern recognition layer is equal to the number of learning samples. Generally, the number of neurons in the summation layer is two, which used to calculate the weighted output sum of the neurons of the pattern recognition layer S and the pattern recognition layer unweighted output D. The activation function of the pattern recognition layer neurons is as shown in equation (1).

$$G_i(x) = \exp[-\frac{(X-X_i)^T(X-X_i)}{2\sigma^2}] \quad (1)$$

The output of the pattern recognition layer neuron i is an exponential form of the square of the Euclid distance between the input variable and it's corresponds sample X. X is the network input variable; X_i is the sample of the learning corresponding to the i-th neuron.

The summation formulas of the two neurons in the summation layer are:

$$S = \sum_{i=1}^{n} Y_i \exp(-\frac{(X-X_i)^T(X-X_i)}{2\sigma^2}) \quad (2)$$

$$D = \sum_{i=1}^{n} \exp(-\frac{(X-X_i)^T(X-X_i)}{2\sigma^2}) \quad (3)$$

In the above formula, Y_i is the weight that connects the i-th neuron of the recognition layer to the summation layer, and σ is the smoothing factor.

Generalized Regression Neural Networks is a powerful tool for nonlinear regression analysis. For the input vector X, the output Y of the generalized regression neural network is calculated by the following function:

$$Y(X) = \frac{S}{D} = \frac{\sum_{i=1}^{n} Y_i \exp(-\frac{(X-X_i)^T(X-X_i)}{2\sigma^2})}{\sum_{i=1}^{n} \exp(-\frac{(X-X_i)^T(X-X_i)}{2\sigma^2})} \quad (4)$$

Generalized regressive neural network is a variation of RBF neural network and often used for function approximation [12]. The generalized regression neural network can adjust the number of hidden layer neurons. The more neurons in the hidden layer, the more accurately the approximation is. Therefore, generalized regression neural networks have more advantages than the ordinary RBF neural networks.

2.2 The principle of Kriging interpolation

Kriging predicts the value of a function at a given point by calculating the weight average of the values of the sample points of the function in the neighborhood of the point. Kriging interpolation is a linear undeviated optimal estimation interpolation method, which not only considers the positional relationship between the observation point and the estimation point fully, but also considers the spatial relationship [13].

According to the principle of Kriging interpolation, if there has the known noise N (0, σ^2) in the simulated model, the known noise can be added to the Kriging interpolation process directly to construct the fitting function Δy. The Kriging interpolation formula is:

$$\Delta \mathrm{y} = \mathrm{GP}(0, \mathrm{K}) + \mathrm{N}(0, \sigma^2) \quad (5)$$

In order to estimate the unknown value of the regional variation, the theoretical model of the variogram needs to be fitted based on the measured observations. The commonly used variogram models including exponential models, spherical models, Gaussian models, and power function models [14]. The Gaussian model can experimentally map the input vector to the nonlinear space and accurately fit the local properties of the function, so the Gaussian model is used in the KGRNN modeling system. The variogram Gaussian model formula is:

$$\gamma(\mathrm{h}) = \begin{cases} 0 & , h = 0 \\ 1 - e^{-(\frac{h}{a})^2} & , h > 0; \end{cases} \quad (6)$$

In the above formula, h represents the Euclidean distance between two sampling points, and a is the range. If the collecting data contains noise, add noise to the variogram, and the variogram of the added noise becomes:

$$\gamma(\mathrm{h}) = \begin{cases} 0 & , h = 0 \\ 1 - e^{-(\frac{h}{a})^2} + \sigma P(x) & , h > 0; \end{cases} \quad (7)$$

P(x) is the probability density of the noise function and σ is the spread factor of the noise function.

2.3 Test function measure

In order to compare the degree of fitting of the experiment and reduce the contingency of the laboratory, multiple experiments were used to average, and the fitted function was evaluated using root mean squared error (RMSE) and the maximum deviation (MAXERROR):

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{N}(y_i' - y_i)^2}{N}} \quad (8)$$

$$\mathrm{MAXERROR} = \mathrm{Max}_{\mathrm{i<N}}|\mathrm{y_i'} - \mathrm{y_i}| \quad (9)$$

N is the amount of data in the test set, y_i' is the response surface prediction value, and y_i is the test function value.

3. KGRNN LEARNING ADJUSTMENT METHOD

The Generalized Regression Neural Network (GRNN) and RBF neural network will produce fluctuation deviation in the fitting. FIGURE 2 is $\mathrm{y} = \mathrm{x} + x^2 + 0.1 \times \sin(0.1 \times x)$ fitting the deviation curve (RBF) in the one-dimensional function of the GRNN. (The neural network fit value minus the true value of the function). In the scaled fitted curve, the curve of the fitted and the curve of the real test function will have different fluctuation values, which is due to the fluctuations in the fitting and it leads to deviation of the function fitting.

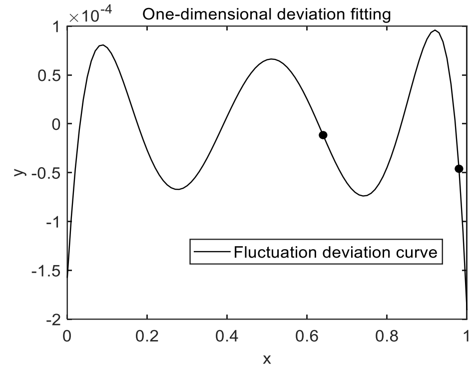

FIGURE 2: One-dimensional generalized

In the section between two blacks [0.64, 0.98] in FIGURE 2, two deviation curves are selected, the variance and the mean of the normal distribution are calculated by using the deviation value to draw a normal distribution as shown in FIGURE 3, which in the calculated. The variances are [0.006, 0.002], and the mean values are [0.75, 0.92]. It can be seen that the deviation is a similar normal distribution. Such the properties are also used in multivariate normal distributions, because the multivariate normal distribution is a mathematical extension of the normal distribution. The Gaussian process, which is an extension from the multidimensional Gaussian distribution to the infinite dimension. every point of the input space is associated a random variable subject with a Gaussian distribution. The joint probability of a combination of any finite number of these random variables is also subject to a Gaussian distribution. While Kriging is a Gaussian process regression, it used the priori covariance, so Kriging interpolation can fit the multivariate normal distribution well, and the fluctuation of the normal distribution can be well fitted in the Kriging interpolation.

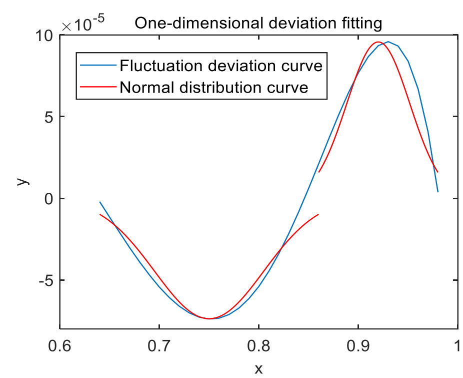

FIGURE 3: Fluctuation deviation of the normal distribution

In the multi-dimensional function fitting, the symmetric deviation is represented by the multivariate normal distribution in the high-dimensional space, and the deviation in each dimension of the fitted region can be expressed in the mathematical formula $\mathrm{N}(\mu = \mathrm{x}, \sigma^2)$.

3.1 Preprocess the collected data

The test functions of the constructed surrogate model are complex functions with multiple peaks and valleys. In the fitting interval, the method of Latin hypercube sampling is generated random sampling data of normal distribution, which is eliminate the deviation in the fitted area. Assuming that all data sets are D, then the first part of the training set traindata1= {(x1, y1)|(x1,y1) ∈D} is extracted in the total data set D, and the generalized RBF neural network is trained. Then the second part of the training data is traindata2={(x2,y2)|(x2,y2)∈S},which S is remaining data set S(S =D-traindata1) . This part of the data is used as the center point of the Center point of radial-based neurons. Finally, the test set testdata={(x1,y1)|(x1,y1)∈(testdata)} is extracted from the remaining data sets.

3.2 KGRNN calculation description

The calculation process of the constructed KGRNN modeling system is shown in FIGURE 4. The figure shows three processes of fitting calculation of KGRNN modeling system. These three processes are extracting GRNN fitting deviation, Kriging interpolation fitting deviation and GRNN eliminate deviation.

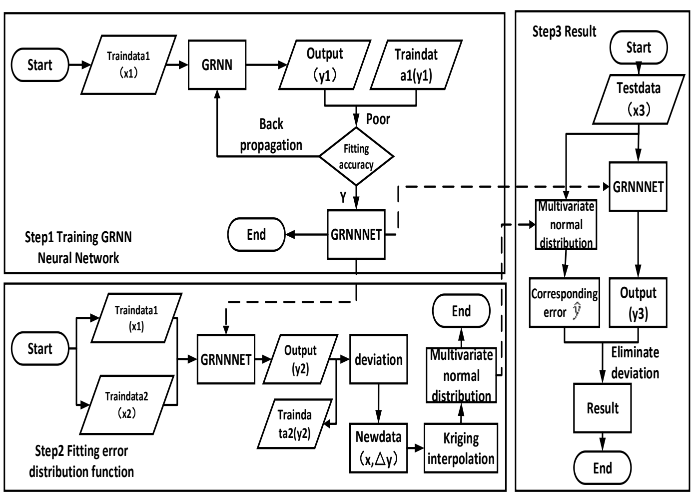

FIGURE 4: KGRNN modeling system

3.2.1 Extracting GRNN to fit fluctuation deviation

The radial basis function selects the Gaussian function because the Gaussian function can map the input vector to the nonlinear space and accurately fit the local properties of the function. Using the generalized regression neural network from better performance to control the number of hidden layer neurons freely.

In this article, the generalized regression neural network fluctuation deviation is the most important part. The extraction error is important to collect different data through the different data sets, then calculate the data of every part to get the deviation of the required solution. Firstly, the extraction in the collected dataset is trained on the generalized regression neural network by using the above traindata1 set. The trained neural network is substituted into the generalized regression neural network trained using traindata1 and traindata2, then iterated in the generalized regression neural network. The generated new data set outputdata = {(x2, y2') | (x2, y2')}.

The predicted value y2' generated by the GRNN in the newly generated dataset outputdata minus the value y2 of the training set of the sample in the training dataset traindata2 can be approximated as the fluctuation deviation y in the entire fitting interval. The datasets involved in the training of GRNN were shown in the FIGURE 3 as the two ends of the fluctuation deviation. It is assumed that the deviation of the data participating in the generalized regression neural network training is zero, the two partial deviation values and the sampled the input values are combined into the fitted deviation set newdata, the resulting deviation can be considered as an approximate fluctuation deviation over the entire fitting interval. It is sure that the approximate fluctuation deviation has a direct relationship with the collected data distribution. In order to ensure the accuracy of the final fitting, the above training data set is required to be randomly and distributed throughout the fitting interval evenly.

3.2.2 Kriging interpolation fitting deviation

Through the iterations of different training sets, the approximate deviation set of the generalized regression neural network is extracted. Then the deviation set is brought into the Kriging interpolation to calculate the deviation distribution function.

As the following shown in FIGURE 5, the deviation fluctuation is constructed in the fitting interval of the two-dimensional Ackley test function. When the GRNN is used for function fitting, the fitting on the fitting boundary is seen from the image, which is a big fluctuation.

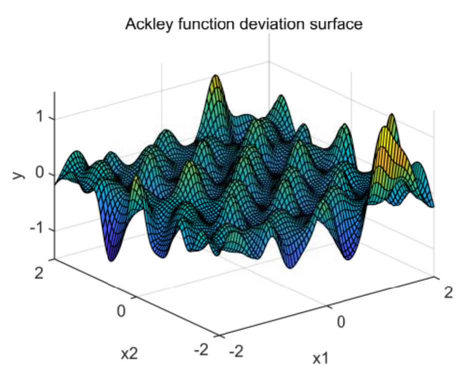

FIGURE 5: Fluctuation deviation of 2D Kriging construction

3.2.3 GRNN eliminate deviation

Kriging interpolation is used to solve the deviation distribution function of the generalized regression neural network. After the generalized regression neural network trained by traindata1, and the Kriging deviation term also added to eliminate the fluctuation deviation of the generalized regression neural network in the fitting.

At the point of this, the entire KGRNN modeling model is completed. The calculation process of Kriging is the same as the calculation procedure of the second section. Finally, the test data set testdata is used to verify the fitting effect of the KGRNN modeling model.

3.3 Experimental comparison analysis and noise processing capability

3.3.1 Comparison of different test functions

In order to verify the accuracy of the KGRNN construction, the methods of KGRNN, KRBF, GRNN, Kriging, and RBF response surfaces were compared. The KRBF surrogate model in the comparative experiment is the feature of the RBF neural network fitting function. The error of the Kriging fitting function and the error is subtracted from the fitted RBF neural network model. The training set and test set of Kriging and GRNN neural networks are traindata1 ∪ traindata2 and testdata respectively. For experimental accuracy, the five surrogate models, which is used diffident test functions, is used the same training set and the test set. The experimental platform is MATLAB2018B and CPU: i7700HQ and GPU: GTX1050Ti.

In order to analyze the performance of the KGRNN modeling system, these five different test functions were selected to perform performance analysis on the KGRNN modeling system. The five test functions (TF) which is used therein are respectively Ackley Function (AF), Himmelblau function (HM), Leon's function (LF), Schaffer's Function (SF) and Six-hump Camel Back function (SHCF). The function settings include the sampling interval (Domain), the number of hidden layer neurons (NH) of the RBF neural network in the comparison experiment and the number of input training data (Data set) as shown in the following Table 1. In order to verify the accuracy of the experiment, also reduce the error caused by a single experiment, the experimental test uses 100 experimental results to solve the average value as the final experimental result.

Table 1: Setting test function parameters

TF	NH	Domain	Data set		
			Traindata1	Traindata2	Testdata
AF	40	[-2 -2;2 2]	50	50	1000
HM	15	[-3 -3;3 3]	20	20	1000
LF	15	[-2 -2;2 2]	20	20	1000
SF	40	[-2 -2;2 2]	40	40	1000
SHCF	20	[-2 -2;2 2]	20	20	1000

Table 2: test function RMSE

TF	KGRNN	KRBF	GRNN	Kriging	RBF
AF	**0.548**	0.679	0.575	0.601	0.754
HM	**2.001**	4.014	14.09	5.600	16.28
LF	**0.035**	0.065	0.101	0.113	0.119
SF	**0.021**	0.060	0.067	0.086	0.067
SHCF	**0.917**	4.312	7.638	4.797	8.159

Table 3: test function Maximum deviation

TF	KGRNN	KRBF	GRNN	Kriging	RBF
AF	**1.736**	2.479	1.736	1.645	2.915
HM	**15.00**	26.44	62.94	9.293	83.79
LF	**0.259**	0.569	0.625	0.261	0.787
SF	**0.022**	0.063	0.774	0.021	0.802
SHCF	**7.485**	28.49	37.27	7.587	44.58

Table 4: test function Running time

TF	KGRNN	KRBF	GRNN	Kriging	RBF
AF	**0.069**	0.160	0.032	0.033	0.120
HM	**0.065**	0.098	0.033	0.020	0.070
LF	**0.063**	0.109	0.034	0.020	0.080
SF	**0.071**	0.172	0.034	0.026	0.132
SHCF	**0.066**	0.095	0.032	0.022	0.076

From the experimental data in Table 2, the fitting function of the KGRNN modeling system is more accurately than the simple RBF neural network and the Kriging interpolation. In the different functions, the KGRNN modeling system is the best fit among the five surrogate models. From the experimental bold data in Table 3, the maximum deviation of KGRNN modeling is also very well. Compared with RBF neural network and KRBF, KGRNN modeling system is suppresses the fluctuation of deviation effectively. This way can reduce the maximum deviation and improve the precision of the fitting function.

Table 4 is the time for counting the calculations of the three surrogate models. It can be seen from the time when the simulation model is established in the table that KGRNN runs for half of the time calculated by KRBF. Such running time has the application of KGRNN simulation model in complex engineering modeling.

3.3.2 KGRNN's ability to handle noise

In order to test whether the KGRNN has ability to reduce noise or not, you can judge by adding different intensity noise and observing the fitting accuracy of the system. The AF function is selected as the fitting object, the Gaussian noise is added to the AF test function as $N(\mu = 0, \sigma^2)$ and the average value of the added noise is zero. As the following shows in FIGURE 6, which is a noise distribution graph with variance radius σ=0.01.

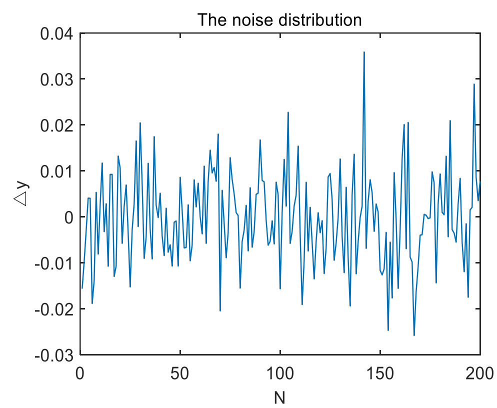

FIGURE 6: Distribution of noise at σ = 0.01

Adding different noises in the AF intensity, the fitted curve is showing in FIGURE 7. In the curve of KGRNN in the figure, we can see that the KGRNN function fitting has strong noise reduction ability. At the same intensities, the noise reduction of KRBF and Kriging interpolation has greater volatility. Compared with KGRNN, it has a very smooth noise reduction capability for different intensity noise. Because almost all of sampling will contain a part of the noise, which is difficult to be applied in practical engineering without the certain noise reduction ability. In summary, the KGRNN modeling system has a certain noise reduction capability, which enhances the accuracy of KGRNN in function fitting and improves the robustness of the simulation model.

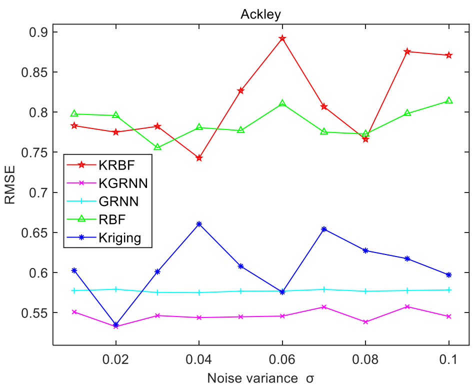

FIGURE 7: Different intensity noise fitting graph

4. KGRNN SIMULATION COMPOSITE SHEET DEFLECTION

The deflection of square composite panels is an important analysis in the structural optimization design. In order to verify the correctness of the modeling model, the KGRNN modeling system is used to approximate this response surface model. According to the literature [15], the global deflection is determined by six different variables and four of them are geometrical variables of composite sheets, which shown in FIGURE 8. Table 5 is a description of each variable and a boundary value.

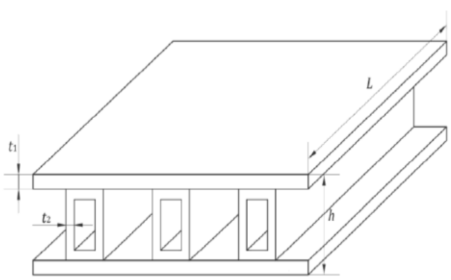

FIGURE 8: Square composite sheet

Table 5: Description of square composite deflection variables

Variable name	Variable description	Min value	Max value	Unit
L	Sheet length	3	7	m
h	Sheet height	4	16	mm
t_1	Upper and lower metal plate thickness	4	4	mm
t_2	Intermediate rib thickness	2	4	mm
k_n	Intermediate rib spacing factor	1.5	4	
n	Number of intermediate ribs	1.5	6	

In the finite element analysis, the bottom of the square composite sheet is a simply supported beam. A uniform load of 3 kPa was loaded on the top of the composite metal composite sheet, and the center was loaded with a concentrated load of 1 KN. Using ANSYS analysis, the node SHELL is 181 units, and 500 sets of simulation results are collected.

Table 6: Average simulation results of modeling system deflection

	KGRNN	KRBF	GRNN	Kriging	RBF
RMSE	$\mathbf{1.8\times10^{-4}}$	$2.5\times\mathbf{10^{-3}}$	$2.2\times\mathbf{10^{-3}}$	$2.1\times\mathbf{10^{-3}}$	$2.6\times\mathbf{10^{-3}}$
MAX	$\mathbf{1.6\times10^{-2}}$	$1.8\times\mathbf{10^{-2}}$	$1.7\times\mathbf{10^{-2}}$	$1.5\times\mathbf{10^{-2}}$	$1.9\times\mathbf{10^{-2}}$

From the collecting 500 sets of simulation results, 200 groups were selected to construct the surrogate model, and the remaining 300 sets of experimental results were used to test the accuracy of the modeling systems such as KGRNN, KRBF, GRNN, Kriging and RBF. In order to increase the credibility of the experiment, the average result of the experimental data of 100 repetitions was used as the approximation accuracy of the final fitting model. Table (6) is a comparison of the average RMSE and the maximum deviation (Max Error) of the response surface. As can be seen in the Table (6), the average accuracy of the KGRNN modeling system is the best. It shows that the KGRNN modeling system can establish the response surface model in engineering.

5. CONCLUSION

From the experimental results, the KGRNN modeling system has a great fitting effect on many functions. The fitting experiment which is used five surrogate models and different test functions found that KGRNN had the best fitting effect. At the same time, the KGRNN modeling system has the noise reduction property, the model has the better precision in the system with noise. In the final engineering example, the KGRNN modeling system can also simulate the engineering model, which can meet the accuracy of engineering requirement.

In summary, the KGRNN system is used the generalized regression neural network and the Kriging interpolation principle. Which can reduce the fluctuation deviation generated by the generalized regression neural network in the modeling and improve the accuracy of the function fitting.

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