The ensemble of surrogate model based on local and global errors

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Abstract. The weight coefficient is the key factor for the success of the ensemble of surrogate model construction. In this paper, a method for constructing ensemble of surrogate model by combining local and global errors to calculate weight coefficient has been put forward. Radial basis function (RBF) and the Kriging model are built as the meta models, and the cross validation strategy is applied to calculate the global errors and the local errors of samples. The inverse proportion average method is used to calculate the weight coefficient by combining the local errors and global errors. In order to verify the effectiveness of the proposed method, two meta models and three methods to construct the ensemble of surrogate models are tested with six benchmark functions. The results show that the proposed method can improve the accuracy, robustness and universality of the surrogate model.

1. Introduction

In large-scale engineering optimization problems, because of the huge calculation or unknown performance function, people often use surrogate model for approximate calculations. So the surrogate model has been widely used in engineering optimization problems. The basic principle of the surrogate model is to use interpolation or fitting techniques to replace complex or unknown functions under certain accuracy conditions. The commonly used surrogate models (meta models) include Kriging model [1], radial basis function model [2], polynomial response surface model [3], artificial neural network model [4], and support vector regression model [5], etc. However, for specific complex engineering problems, finding a suitable surrogate model is a difficult task. In order to improve the adaptability of the surrogate model, a reasonable choice is to use a linear combination of multiple meta models, that is, the ensemble of surrogate model. It is expected that the ensemble of surrogate model has better prediction accuracy in the case of linear or nonlinear, low-dimensional or high-dimensional situations. Huang [6] found that the ensemble of surrogate model not only has higher prediction accuracy than meta surrogate model, but also promotes the search for the optimal solution. The research by Jianguang [7] showed that the ensemble of surrogate model can obtain the optimal solution with smaller errors. Pan Feng [8] applied the ensemble of surrogate model to the lightweight design of the car body, and achieved a better optimization effect than the meta surrogate model, Liu Xing [9] applied the ensemble of surrogate model in the structural optimization of the body parts and also achieved better optimization results.

Although the research on the ensemble of surrogate model has made some progress, the technology of current ensemble of surrogate model still has the following shortcomings: 1) The weight coefficient calculation of most existing ensemble of surrogate models mainly depend on the global prediction accuracy of each meta surrogate model [10-11]. 2) The main weight coefficient
calculation methods are computationally intensive, which has complex logic without practical theoretical basis [12-14]. 3) The robustness and universality usually are not considered when evaluate the performance of the ensemble of surrogate model [15-16]. Aiming at the above-mentioned shortcomings of the ensemble of surrogate model, by comprehensively considering the local and global errors, this paper proposes a method to calculate the weight coefficient, and puts forward a new viewpoint to measure the robustness of the ensemble of surrogate model by using the variance of the determination coefficient.

2. The analysis of traditional ensemble of surrogate model

2.1 The ensemble of surrogate model

The expression of the ensemble of surrogate model is:

\[ \hat{y}_e(x) = \sum_{i=1}^{N} \omega_i \hat{y}_i(x) \]  

(1)

where \( \sum_{i=1}^{N} \omega_i = 1 \), \( \hat{y}_e \) is the predicted response of the ensemble of surrogate model, \( N \) is the number of meta models, \( \omega_i \) and \( \hat{y}_i \) are the weight coefficient and predicted response values of the ith meta model, respectively.

There are two key factors to construct the ensemble of surrogate model. The first factor is the selection of meta models, and the second one is the calculation of the corresponding weight coefficients of each meta model. Generally speaking, the higher the prediction accuracy, the greater the weight coefficient of the corresponding meta model.

2.2 Selection of meta model

At present, there are three meta models used in the general ensemble of surrogate model: polynomial response surface (PRS), radial basis function (RBF) and Kriging model. According to the existing data [3], the advantages of polynomial response surface model include less calculation, high linear fit, and simple structure. JIN [17] pointed out that RBF fits the higher-order nonlinear problems better, and the Kriging model is suitable for lower-order nonlinear problems. In recent years, support vector machine model and artificial neural network model have been used in the field of artificial intelligence. Because of their immature development and low accuracy, they are rarely used in surrogate models.

2.3 The calculation of weight coefficient

At present, the most commonly used method to calculate the weight coefficient of the ensemble of surrogate model is the combination of multiple meta models (PRS, Kriging, RBF, etc.). ZARPA [10] calculates the proportion of each meta model in the ensemble of surrogate model by using inverse method that uses the global errors as a measure tool. The commonly used global error indicators are Root Mean Square Error (RMSE) and Generalized Mean Square Cross Validation Error (GMSE). This method is the most commonly used method in the calculation of the weight coefficient of the ensemble of surrogate model. But its prediction accuracy is low. The new weight coefficient calculation method constructed in this paper is innovative and improved on based on inverse method.

3. The Ensemble of surrogate model based on local and global errors

3.1 Meta model selection

In terms of meta-model selection, this paper has selected the radial basis function (RBF) and the Kriging model as the meta-models. The reason why the polynomial response surface model (PRS) is not selected is because more than 90% of engineering problems are nonlinear problems, and PRS is suitable for linear problems, and the fitting performance in nonlinear problems is poor. RBF and Kriging models have two complementary advantages, which can be applied to different situations
such as low-dimension and high-dimension, low-order and high-order, etc. The ensemble of surrogate model can make full use of these advantages. In addition, more meta models do not mean better predict accuracy.

3.2 Improved weight coefficient algorithm
Different from the existing calculation methods of weight coefficients, the weight coefficient algorithm proposed in this paper comprehensively considers local and global errors, which takes local errors into account in order to expect good prediction accuracy and robustness.

The traditional method of calculating the weight coefficient of the ensemble of surrogate model has always used the global error as a measure. The traditional method to calculate the weight coefficient is as follows:

$$\omega_i = \frac{1}{\sum_{j=1}^{N} V_j}, \quad \sum_{i=1}^{N} \omega_i = 1$$  \hspace{1cm} (2)

where the $V_i$ is the predicted variance of the ith meta-model. The predicted variance $V_i$ can be calculated directly by RMSE, which can be expressed as follows:

$$V_i = \text{RMSE} = \frac{1}{\sqrt{n}} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$  \hspace{1cm} (3)

where $n$ is the number of samples, $y_i$ and $\hat{y}_i$ are the actual and predicted values of the ith sample, respectively. When calculate the weight coefficients, the relationship between the local error and the global error of each meta-model should be considered comprehensively. The global error measurement index of the surrogate model is the root mean square error (RMSE), and the measurement index of the local error is the maximum absolute error (MAE). The calculation formula is as follows:

$$\text{MAE} = \text{Max} |y_i - \hat{y}_i|$$  \hspace{1cm} (4)

In the weight coefficient algorithm combining local and global precision proposed in this paper, the weight coefficient is defined as:

$$\omega_i = \frac{1}{\sum_{j=1}^{N} T_j} \quad (i = 1, 2), \quad \sum_{i=1}^{N} \omega_i = 1$$  \hspace{1cm} (5)

$$T_i = \text{RMSE} + \alpha \text{MAE} \quad (0 < \alpha < 1)$$  \hspace{1cm} (6)

where the value of $\alpha$ is a key. Since there is no systematic research on the value of $\alpha$, three values of 0, 0.5 and 1 are selected as alternative values. If the value of $\alpha$ is greater than 1, it will overemphasize the importance of local accuracy. However, most engineering problems still need to ensure the global accuracy of the ensemble of surrogate model. It is worth mention that when $\alpha$ equals to 0, the local error of the surrogate model is not taken into account, the weight coefficient calculation method proposed in this paper actually is the classic inverse proportional averaging method.

3.3 Evaluation index of ensemble of surrogate model
The evaluation index of the prediction accuracy and robustness of the ensemble of surrogate model adopted in this paper is the determination coefficient. The specific expression is as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^{N} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{N} (y_i - \bar{y})^2}$$  \hspace{1cm} (7)
\(\bar{y_i}\) is the average of the actual response values. Both the root mean square error (RMSE) and the determination coefficient \((R^2)\) can reflect the global accuracy of the surrogate model, but RMSE is greatly affected by the specific case, and cannot directly reflect the errors. When the error is normalized, the closer the value of \(R^2\) is to 1, the higher the accuracy of the surrogate model, which is intuitive and easy to understand.

At the same time, since the accuracy value of the meta surrogate model in a test case does not fluctuate much, we do not use the traditional box diagram to evaluate the robustness of the surrogate model. In order to observe the robustness of constructed the ensemble of surrogate model, the variance of the determination coefficient is used to visually observe the subtle changes.

3.4 Main steps of the improved ensemble of surrogate model

The specific process of the improved ensemble of surrogate model is shown in Figure 1.

![Flowchart of model construction](image)

Figure 1. Flowchart of model construction.

1) Generate the samples. Latin hypercube sampling [19] is applied in this paper, which can ensure the randomness and uniformity of sampling. After obtaining the samples, the real response values of samples can be obtained by using simulation methods.

2) Establish the meta models. Establish the RBF and the Kriging models by using the data of samples. Then cross-validate method (CV verification) [20] is used to obtain the average square root error (RMSE) and maximum absolute error (MAE), which are used to measure the local and global errors of the surrogate model, respectively.

3) Use the weight coefficient calculation method proposed in this paper to calculate the weight coefficients when the values of \(\alpha\) are 0, 0.5 and 1, respectively. Then the ensemble of surrogate models can be constructed.

4) Verify the prediction accuracy and robustness of the ensemble of surrogate models.

4. Benchmark function verification
4.1 Benchmark functions

The 6 representative benchmark functions from the standard test function library [21] are selected, which can represent low-dimension and high-dimension, low-order and high-order situations. The specific expressions are shown in Table 1.

Table 1 Benchmark functions.

| Function number | Study expression |
|-----------------|------------------|
| 1               | $y = x_1 e^{x_1 + x_1^2} + x_1, x_1 \in [-2, 2]$ |
| 2               | $y = 2x_1^2 - 1.05x_1^4 + \frac{x_1^6}{6} + x_1x_2 + x_2^2, x_1 \in [-5, 5]$ |
| 3               | $y = (x_1^2 + \frac{5}{4}x_1^2 + \frac{5}{8}x_1^6 - 6)^2 + 10(1 - \frac{1}{8\pi})\cos(x_1 + 10)$ |
|                 | $x_1 \in [-5, 10], x_2 \in [0, 15]$ |
| 4               | $y = 10\sin(2(x_1 - 0.6x_2)) + x_1 + x_2 + x_1x_2 + x_1x_2 + x_1x_2 + x_1x_2$ |
|                 | $x_1 \in [0, 1]$ |
| 5               | $y = \sum_{i=1}^{3} \frac{x_1}{10} \sin\left(\frac{16}{15}x_1 - 1\right) + \sin\left(\frac{16}{15}x_1 - 1\right)$ |
|                 | $x_1 \in [-1.1]$ |
| 6               | $y = \sum_{i=1}^{3} \frac{x_1}{10} \sin\left(\frac{16}{15}x_1 - 1\right) + \sin\left(\frac{16}{15}x_1 - 1\right)$ |
|                 | $x_1 \in [-1.1]$ |

4.2 Comparative analysis of prediction accuracy and robustness

For the six benchmarks, two meta models (RBF and Kriging) and three ensembles of surrogate models corresponding to different $\alpha$ values are established. In Table 2, MUL stands for the ensembles of surrogate model. The values of the ensembles of surrogate model with the highest prediction accuracy is shown in Table 3.

| Function number | $R^2$ | RBF     | Kriging  | MUL   |
|-----------------|-------|---------|----------|-------|
|                 |       | Mean    |          | $\alpha=0$ | $\alpha=0.5$ | $\alpha=1$ |
| 1               |       | 0.89217 | 0.99425  | 0.99457 | 0.99705 | 0.99704 |
|                 | variance | 4.2e-3 | 7.5e-5  | 1.8e-5 | 3.5e-6 | 1.1e-5 |
| 2               |       | 0.91830 | 0.99563  | 0.9938  | 0.99418 | 0.9932 |
|                 | variance | 7.4e-4 | 1.2e-4  | 4.4e-5 | 2.3e-5 | 4.3e-5 |
| 3               |       | 0.88328 | 0.99159  | 0.98390 | 0.9853 | 0.97972 |
|                 | variance | 4.8e-3 | 8.3e-5  | 2.6e-4 | 2.4e-4 | 1.4e-3 |
| 4               |       | 0.98817 | 0.98978  | 0.99364 | 0.99423 | 0.99667 |
|                 | variance | 3.2e-5 | 8.1e-5  | 1.1e-5 | 1.2e-5 | 1e-5 |
| 5               |       | 0.99898 | 0.93990  | 0.99867 | 0.99845 | 0.99991 |
|                 | variance | 7e-8  | 1.6e-2  | 2.2e-7 | 2.8e-7 | 1.8e-7 |
| 6               |       | 0.99846 | 0.82923  | 0.99485 | 0.99736 | 0.99721 |
|                 | variance | 1.1e-7 | 1.5e-3  | 3.6e-4 | 7.8e-7 | 9.3e-7 |

Table 3 Corresponding minimum errors of benchmark functions.

| Function number | Minimum error | $\alpha$ |
|-----------------|---------------|----------|
| 1               | 0.00280       | 0.5      |
From Table 2 and Table 3, we can see that:

1). From the perspective of prediction accuracy, the benchmark functions can be divided into two categories. The first category is that the prediction accuracy of the meta models are lower than that of the ensembles of surrogate model. Taking function 1 as an example, it can be seen from the mean of the determination coefficient that the Kriging model has the highest prediction accuracy of two meta models. Among the three ensembles of surrogate models, the one with the highest prediction accuracy is the ensemble of surrogate model when $\alpha = 0.5$. The mean value of its determination coefficient is 0.99705. The results of functions 4 and 5 are similar to those of function 1. The second category is that the prediction accuracy of one meta model is slightly higher than that of any ensemble of surrogate model. Taking function 6 as an example, the RBF model has the highest prediction accuracy that the mean of determination coefficient is 0.99846. Among the three ensembles of surrogate model, the highest prediction accuracy is the ensemble of surrogate model at $\alpha = 0.5$ that the mean of the determination coefficient is 0.99736. Although the prediction accuracy of one meta model is slightly higher than that of any ensemble of surrogate model, the difference in accuracy between these two types is not large. The results of functions 2 and 3 are similar to those of function 6. In general, the prediction accuracy of the ensemble of surrogate model is higher.

2). From the perspective of robustness, the results of test examples are also divided into two categories. The first category is that the robustness of the meta surrogate model is lower than that of the ensemble of surrogate model. Taking function 1 as an example, it can be seen from the size of the variance of the determination coefficient that the meta surrogate model with the strongest robustness is the Kriging model, and the variance of the determination coefficient is the smallest with a value of 7.5e-5. Among the three ensembles of surrogate models, the most robust ensemble of surrogate model is the ensemble of surrogate model when $\alpha = 0.5$, which has the smallest variance of the determination coefficient with a value of 3.5e-6. The results of Example 4 and Example 5 are similar to those of function 1. The second type takes function 6 as an example. The meta model with the strongest robustness is the RBF model, whose decision coefficient has the smallest variance of 1.1e-7. Among the three ensemble of surrogate models, The strongest is the ensemble of surrogate model at $\alpha = 0.5$, with the smallest variance of the coefficient of determination with a value of 7.8e-7. Although the robustness of the meta surrogate model is slightly stronger than that of the ensemble of surrogate model, they are not much different. The results of function 2 and function 3 are similar to function 6. On the whole, the ensemble of surrogate model is more robust.

It can also be seen from the above comparison results:

1). For the meta model, in terms of prediction accuracy, in the case of less than four dimensions, the radial basis function (RBF) has lower prediction accuracy than the Kriging model, and the Kriging model has obvious advantages. In terms of robustness, when the dimension is lower than 4, the robustness of the Kriging model is higher than the radial basis function; when it is higher than four dimensions, the robustness of the RBF model is superior to the Kriging model.

2). It can be seen from Table 3 that the prediction accuracy of the ensemble of surrogate model has been improved to some extent by using the algorithm of combining local and global errors proposed in this paper. Compared with the surrogate model constructed by the meta surrogate model and the traditional inverse proportional averaging method ($\alpha = 0$), the prediction accuracy of the ensemble of surrogate model after taking into account local errors has been further improved, which is more conducive to later optimization and the robustness improvement.
4.3 Comparative analysis of universality

In addition to consider the prediction accuracy and robustness of each surrogate model in different test problems, its universality must also be considered. The universality is used to evaluate the fluctuation of the prediction accuracy of the surrogate model in different test cases. From low dimensional problems to high dimensional problems, in order to facilitate comparison, the results are expressed in the form of box figure [22]. The decision coefficients of each surrogate model in this paper are shown in Figure 2. MUL0, MUL0.5, and MUL1 correspond to the ensemble of surrogate models with values of $\alpha = 0, 0.5, \text{and } 1$, respectively. It can be seen from the figure that in the six test cases, the two meta surrogate models have too large a distance between the upper and lower ends of the rectangle compared to the three ensemble of surrogate models, the universality is not strong. The universality of radial basis function (RBF) model is the worst, followed by the Kriging model. The universality of the three ensemble of surrogate models is stronger than that of the meta surrogate model, but the universality of the three ensemble of surrogate models is very close.

![Figure 2. Universality of decision coefficients of each surrogate model.](image)

5. Conclusion

This paper analyzed the shortcomings of the traditional ensemble of surrogate model. An improved ensemble of surrogate model construction method is proposed that combines the local and global errors to calculate weight coefficients. Through 6 test examples, the proposed method is compared with Kriging model, RBF model and traditional ensemble of surrogate model in terms of accuracy, robustness and universality. The conclusions are as follows:

1) The meta surrogate model cannot adapt to some test cases and engineering problems, and its universality is poor. The ensemble of surrogate model is more universal than the meta surrogate model, and has a wider range of applications. It overcomes the difficulty of choosing a surrogate model for specific engineering problems. At the same time, the accuracy and robustness of the ensemble of surrogate model are better than the meta surrogate model, which can better fit various original functions and black box problems.

2) Compared with the traditional ensemble of surrogate model, the proposed ensemble of surrogate model by combining local and global errors has higher accuracy, and has stronger robustness and better universality.

3) Although the method proposed in this paper can improve the accuracy of the ensemble of surrogate model, the specific value of $\alpha$ is not completely clear, and the problem of the value of $\alpha$ needs to be studied in the future.

Acknowledgments
This research is supported by the National Natural Science Foundation of China under the Contract no. 51975106.

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