STUDY ON THE IMPROVED KRIGING-BASED OPTIMIZATION DESIGN METHOD

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Abstract

The improved Kriging-model-based optimization design method which is combined with design of experiment of Latin hypercube sampling, Kriging model and genetic optimization algorithm is develo ped in this paper. By simultaneousl y adding the sample point with maximum EI (Expected Improvement) and the optimal point from optimization of the initial samples, a new Kriging mo del of high er accuracy is formed gradually, with above measure the optimization of given objective can be realized.

The fitting accuracy of Kriging model based on EI method is investigated and validated through the tests of a one- dime nsional function and an aerodynamic problem, which show that the developed Kriging mo del can be effectively used in objectiv e evalu ations in o ptimization problems.

For construction of the improved Kriging model of the aerodynamic problems, the aerodynamic performances of sample points are evaluated using a Reynolds Averaged Navier-Stokes (RANS) Solver. A drag reduction optimization design of R AE2822 airfoil is carried out for examining the validity and efficien cy of presen t method. The drag coefficient of RAE2822 airfoil is reduced by 33.6%. It s hows that this method can gradually improve the fitting a ccuracy of Kriging m odel, finally achieve the great improvement of aerodynamic performance for the airfoil.

1 Introduction

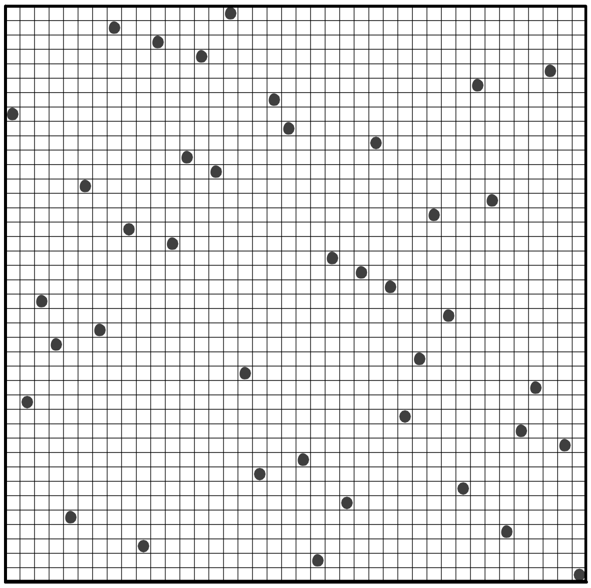
With the development of the computational fluid dynamics (CFD) and the growth in computer's performance, CFD has been used more and more widely in aerodynamic optimization design. The optimization methods usually used today can be classified into two kinds: the gradient-based methods and the non-gradient-methods such as genetic algorithm. The gradient-based optimization methods require the objective function be derivable, and since they need the calculations of the gradients of the objective function with respect to design variables, they call for a large amount of computations when the number of design variables is large, moreover, they have difficulties in finding the global optimum solutions for problems with high nonlinearity, such as aerodynamic problems. Non-gradient-methods such as genetic algorithm have the advantage of being able to find the global optimum point of optimization problems, but the computaion cost is very huge because of the wide searching space of practical aerodynamic problems, hence the applications of this kind of methods in aerodunamic problemes are limited.

In recent years, optimization methods using approximation models gained more and more attention because of their high efficiency and utility. These methods use the approximate models to replace the complex and time consuming experiments or numerical simulation of the opitimization problems. For problems of aerodynamic optimization based on Reynolds Averaged Navier-Stokes (RANS) Solver, the biggest advantage of this kind of method is that the number of the flow solver calling can be greatly decreased via using approximate models. The approximate models which are usually used are response surface model, Kriging model, and radial basis function model and so on. Nowadays these models have been broadly investigated. Because of the high nonlinearity of aerodynamic optimization problem, the precision of the final optimal results greatly rely on the accuracy of the approximate models. In recent yeas, Kriging model has been widely used in aerodynamic optimization design due to its ability to approximate highly nonlinear or multi-extremum problems. Many investigations in aerodynamic optimization design using Kriging model have been studied: Shinkyu J etc[1] developed an aerodynamic optimization design method combining the Kriging model and genetic algorithm, which was applied to a two-dimensional airfoil design and the prediction of flap's position in a multi-element airfoil; Mashiro K etc[2] used the Kriging model in multi-objective optimization design on the elements' settings of the high-lift airfoil; M Sekishiro etc[6] proposed an expected improvement (EI)-based method and obtained good results in searching the extremums of some testing functions, in this method, the sample points derived from EI and optimization algorithm are both added to the initial sample points, then a new model is reconstructed to improve the precision of the Kriging model. In this paper this method is applied to aerodynamic optimization design of airfoils, after particular investigation of the precision of the Kriging model, an improved Kriging-model-based optimization design frame which is combined with the Latin hypercube sampling (LHS), Kriging model and optimization method is developed. A one-dimensional function and an aerodynamic problem are tested to validate the fitting accuracy of the improved Kriging model, the results show the developed Kriging model fit the problems well. By using the RANS Solver as the tool of evaluation sample airfoils' aerodynamic pefermance, a drag reduction optimization design of RAE2822 airfoil is carried out for examining the validity and efficiency of present method.

2 Latin hypercube sampling[5]

Before constructing the Kriging model, a certain amount of sample points should be selected in the design space by certain method of design of experiments (DOE). The methods of DOE which have been usually used are orthogonal arrays, uniform design method and Latin Hypercube Sampling (LHS) etc. LHS, which is a popular modern space-filling method and has been widely utilized, is used to select the sample points in this paper.

The distribution of the sample points using LHS method for two variables (n=2) is shown in the figure 1. Here the range of the variables is [-1, 1], the number of sample points is k. The design space shown in figure 1 is divided into k^n bins (k is the number of sample points, n is the number of variables), and each sample locates in the center of a bin, for all one-dimensional projections of the k samples and bins, there will be one and only one sample in each bin, this fully satisfy the criterion of LHS. This also demonstrates that LHS adopted in this paper is correct and can describe the physical feature of design space.



n=2 k=40

Fig. 1. The distribution of sample points using LHS method

3 Kriging model

The Kriging model expresses the relation between response of the system and variables as

$$y(\vec{x}) = f(\vec{x}) + z(\vec{x}) \qquad (1)$$

Where $y(\vec{x})$ is the unknown Kriging model, $f(\vec{x})$ is the known function dependent on $\vec{x}$, it provides a global model. $z(\vec{x})$ is stochastic process, whose average is zero but variance is not, representing the local deviation from the global model. The covariance of $z(\vec{x})$ is expressed as

$$Cov\left[Z(\vec{x}^i), Z(\vec{x}^j)\right] = \sigma^2 \mathbf{R}\left[R(\vec{x}^i, \vec{x}^j)\right] \qquad (2)$$

where $\mathbf{R}$ denotes the correlation matrix, $R(\vec{x}^i, \vec{x}^j)$ expresses the correlation function between any two sample points $\vec{x}^i$ and $\vec{x}^j$. There are a number of correlation functions, such as exponential function, Gaussian function and spline function. The Gaussian function was applied in this paper, which is expressed as

$$R(\vec{x}^i, \vec{x}^j) = \exp[-\sum_{k=1}^{n} \theta_k \left| x_k^i - x_k^j \right|^2] \qquad (3)$$

where $\theta_k (k = 1, \ldots n)$ denotes the unknown correlation parameters, $\vec{x}_k^i$ and $\vec{x}_k^j$ are the kth components of $\vec{x}^i$ and $\vec{x}^j$ respectively. A constant global model is denoted, then equation (1) becomes

$$y(\vec{x}) = \beta + z(\vec{x}) \qquad (4)$$

The predictor of the approximate model could be written as

$$\hat{y}(\vec{x}) = \hat{\beta} + \vec{r}^T(\vec{x}) \mathbf{R}^{-1} (Y_s - \vec{f}\hat{\beta}) \qquad (5)$$

Where Y_s is the response matrix of samples, $\vec{f}$ is a column vector whose elements are all 1, $\mathbf{R}$ denotes the correlation matrix

$$\mathbf{R} = \begin{pmatrix} R(\vec{x}^1, \vec{x}^1) & \ldots & R(\vec{x}^1, \vec{x}^n) \\ \vdots & \ddots & \vdots \\ R(\vec{x}^n, \vec{x}^1) & \cdots & R(\vec{x}^n, \vec{x}^n) \end{pmatrix} \qquad (6)$$

$\vec{r}(\vec{x})$ denotes the correlation vector between the sample point and the predicting point, which is

$$\vec{r}(\vec{x}) = [R(\vec{x}, \vec{x}^1), R(\vec{x}, \vec{x}^2), \ldots R(\vec{x}, \vec{x}^n)]^T$$

The unknown constant β in Eq.(4) can be obtained using the least square method

$$\hat{\beta} = (\vec{f}^T \mathbf{R}^{-1} \vec{f})^{-1} \vec{f}^T \mathbf{R}^{-1} Y_s \qquad (7)$$

The variance can be obtained as follows:

$$\hat{\sigma}^2 = \frac{(Y_s - \vec{f}\hat{\beta})^T \mathbf{R}^{-1} (Y_s - \vec{f}\hat{\beta})}{N} \qquad (8)$$

The parameter $\vec{\theta}$ in Eq.(3) can be estimated by maximizing the following maximum likelihood function

$$MaxF(\vec{\theta}) = -\frac{N \ln(\hat{\sigma}^2) + \ln|\mathbf{R}|}{2} \quad (\theta \geq 0) \qquad (9)$$

For each $\vec{\theta}$, we can got an interpolation model, the final Kriging model is obtained through finding the optimum $\vec{\theta}$ at which the likelihood function is maximum.

The accuracy of the predictor $\hat{y}(\vec{x})$ depends on the distance from the prediction point $\vec{x}$ to the sample points, the closer point $\vec{x}$ to the sample points, the less error of $\hat{y}(\vec{x})$ is. The root mean square error (RMSE) is expressed as follow:

$$s = \sqrt{s^2(\vec{x})} = \hat{\sigma}^2 \left[1 - \vec{r}^T \mathbf{R}^{-1} \vec{r} + \frac{(1 - \vec{1}^T \mathbf{R}^{-1} \vec{r})^2}{\vec{1}^T \mathbf{R}^{-1} \vec{1}} \right] \qquad (10)$$

4 EI method--- for improving the accuracy of kriging model

As mentioned in the reference [1], though the Kriging model is constructed, there is the possibility of missing the global optimum in the searching space if we rely only on the Kriging model in the process of optimization design, because the model itself includes uncertainty at the prediction point. This will bring great error if the model is not accurate enough, hence we apply the EI method mentioned in the reference [1] and [6] to improve the accuracy of the model. For minimization problems, EI is computed as follows

$$E[I(\vec{x})] = (f_{\min} - \hat{y}) \Phi(\frac{f_{\min} - \hat{y}}{s}) + s\phi(\frac{f_{\min} - \hat{y}}{s})$$

Where $f_{\min}$ is the minimum true objective function value we found, $\hat{y}$ is the Kriging prediction at $\vec{x}$, s is the RMSE of the Kriging model, Φ and ϕ are the standard normal distribution function and normal probability density function respectively. The predicting accuracy of the Kriging model can be improved efficiently by adding the point with maximum EI value to the sample points.

5 Accuracy validation

Once the sample points are selected by LHS method, we can gain the objective value of the sample points using the true function, then the optimum parameters can be obtained by certain optimization algorithm, ultimately, the final Kriging model can be obtained. Figure 2 shows the flowchart of constructing the Kriging model. To test the accuracy of the model, a one-dimensional function is utilized for illustration. Furthermore, an aerodynamic problem is tested to validate the developed kriging model's fitting accuracy.

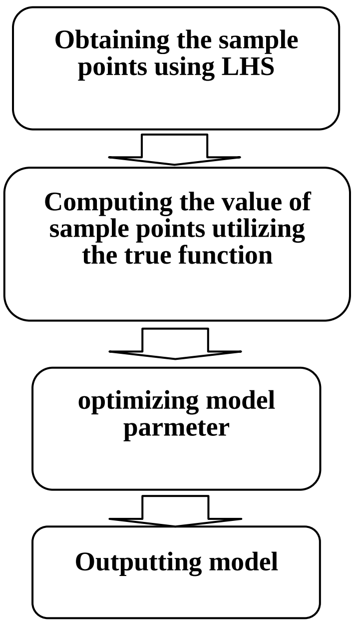
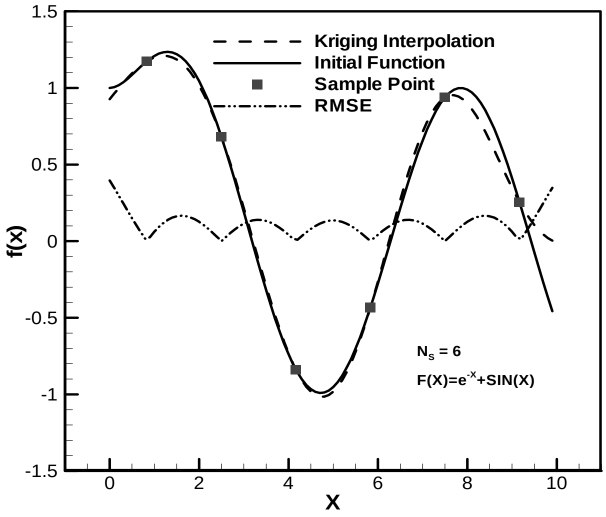


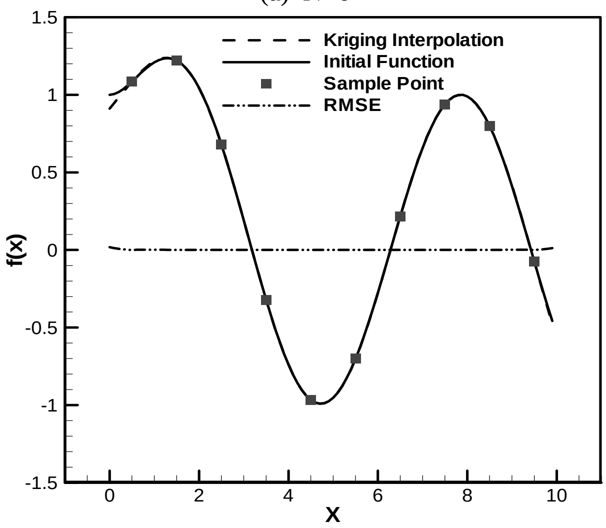
Fig. 2. The flowchart of constructing Kriging model

5.1 Function testing

Figure 3 shows the fitting result of Kriging model for one-dimensional function ($f(x)=e^{-x}+\sin(x)$). The Kriging prediction, true function, sample points and RMSE of the prediction points is given for the number of sample points N equals 6 and 10 respectively. It demonstrates that if the sample points are few (N=6), the approximate model differs clearly from the true function, while the approximation model coincides with the true function quite well if the sample points increase to 10. This means the accuracy of Kriging model is related greatly to the number of samples, that is, the more samples there are, the more accurate the Kriging model is. This can be seen from the RMSE curve likewise. When the sample points are few (N=6), the RMSE at each prediction point is large. We observe that the RMSE at each sample point is zero, just because the Kriging model is the interpolating model, the model passes each sample point precisely. When the number of sample points increases to 10, RMSE at each prediction point approaches zero, this suggests the Kriging model is quite coincident with the true function, so the approximate model is quite accurate.



(a) N=6

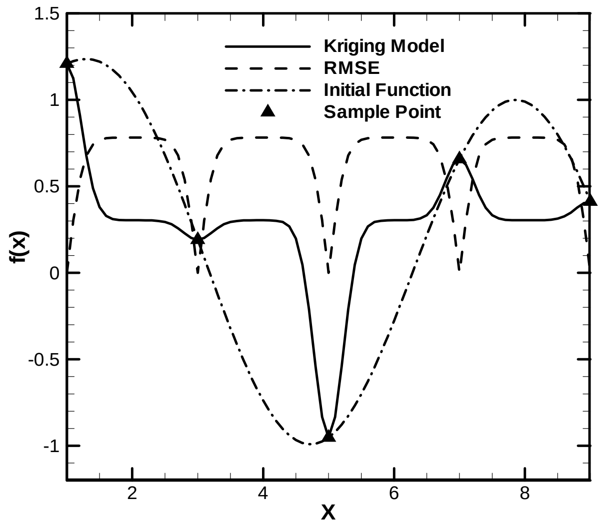


(b) N=10

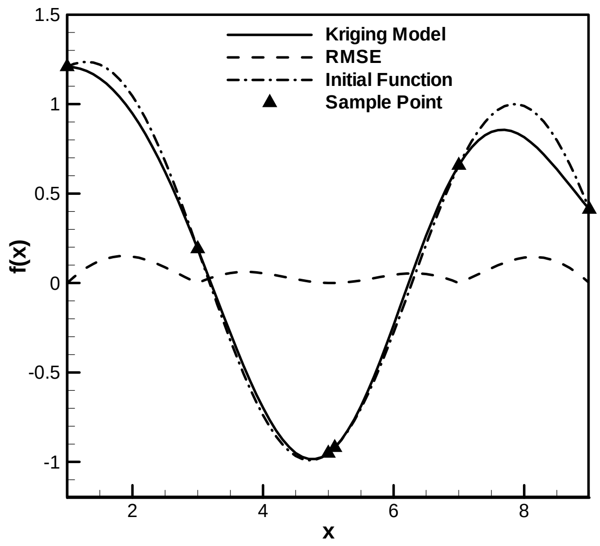
Fig. 3. Schematics of fitting function using Kriging model

Figure 4 shows the process of fitting function using Kriging model after bringing in

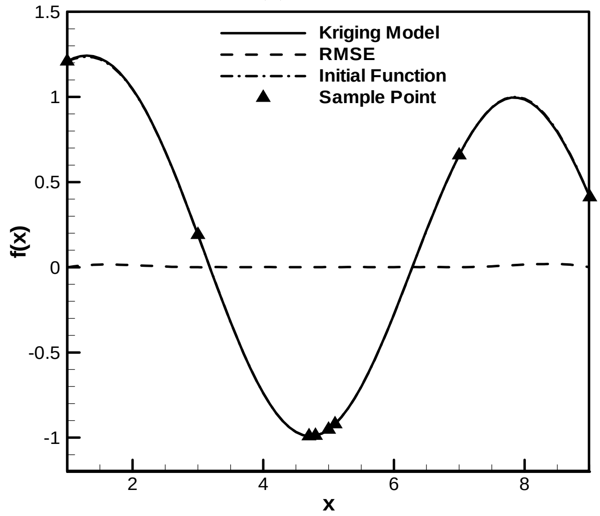
EI method ($f(x)=e^{-x}+\sin(x)$). Five samples are selected initially, we see that the Kriging model differs greatly from the true function, RMSE is large except at the sample points. However, the error of the model could be decreased rapidly through adding a point (the point added can be seen in figure 4(b)) with the maximum EI value , the RMSE is decreased correspondingly, and the accuracy of the Kriging model is increased greatly. With the increase of the sample number, the fitting accuracy of the model is increased correspondingly. When the convergences criterion is achieved, the number of samples reaches 8 (3 samples added, in figure 4(c)), the Kriging model is almost identical with the true function, the RMSE everywhere approaches zero. These illustrate that the model completely satisfies the accuracy requirement. From the results we can conclude: by using the EI-added Kriging model, that is, adding the point at which the EI value is maximum to the former sample points, then reconstructing a new approximate model, we can improve the accuracy of the model remarkably.



(a) N=5



(b) N=6



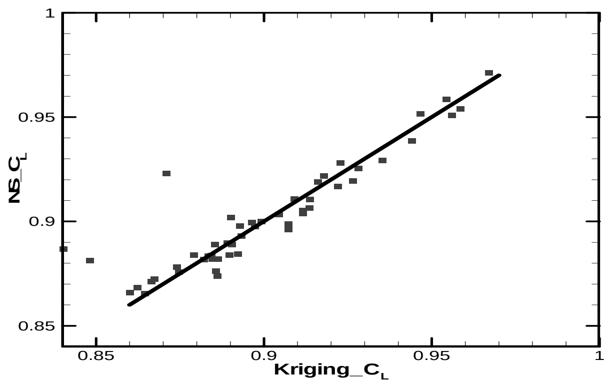
(c) N=8

Fig. 4. The process of constructing Kriging model by bringing in EI method

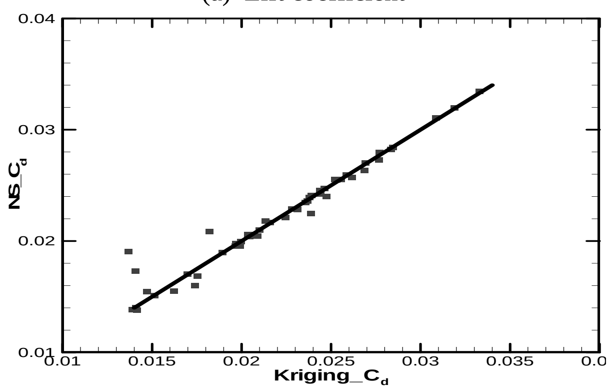
5.2 Aerodynamic problem testing

To validate the predicting power of the Kriging model for aerodynamic problem, an aerodynamic problem is tested. We utilize the RAE2822 airfoil as baseline airfoil, and the Hicks-Henne shape function is adopted to describe the airfoils' geometry perturbation. Firstly, initial samples are selected (N=100) by LHS method, then Kriging model is constructed as before, finally another 50 sample points are selected randomly, and the aerodynamic performance of the airfoil is calculated at each sample point with Kriging model and the RANS Solver (the true value) respectively. The computing results of lift coefficient, drag coefficient and moment coefficient are compared in figure 5 (a)-(c).

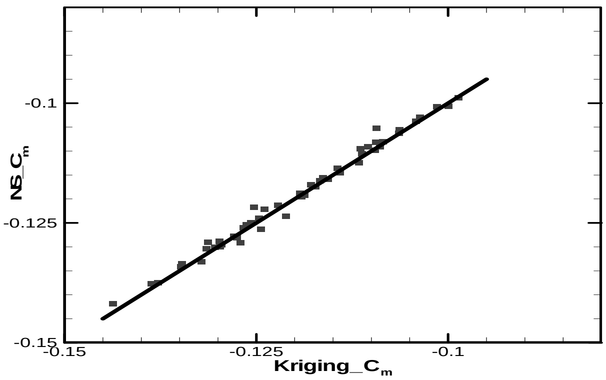
In figure 5 (a)-(c), the solid line denotes that the true values are equal to the predicting values, while the points denote predicting values and the true values, the nearer the point to the solid line, the smaller the prediction error is. Figure 5 (a)-(c) show that the lift coefficient, drag coefficient and moment coefficient at most sample points predicted by Kriging model coincide well with the results got by RANS Solver except for some rare points. The effectivness of the constructed Kriging model for aerodynamic problem is validated. Furthermore, we find that the points with large error in the figure 5(a)-(c) are far from the optimum point, so they almost won't affect the final results of optimization. Consequently, we can conclude that the Kriging model can replace the high fidelity CFD analysis solver to accomplish the process of aerodynamic optimization design.



(a) Lift coefficient



(b) Drag coefficient



(c) Moment coefficient

Fig. 5. Comparison of lift coefficient, drag coefficient, moment coefficient computing from RANS Solver and Kriging model in every sample point

6 Airfoil optimization design

6.1 Framework of Improved Kriging- based optimization design algorithm

The process of the Kriging-model-based optimization design method is described as follows: firstly a number of sample points are generated by method of design of experiments, then the response value at each sample is obtained and the Kriging model is constructed, finally optimization method is used to search the optimum solution. In the searching process, the Kriging model is utilized to calculate the objective function value until the global optimum is obtained. In this paper, the EI method is added to the initial Kriging based optimization design algorithm. According to the reference [6], the optimum point obtained by optimization algorithm is also added to the initial sample points, hence two points are added at a time, then the Kriging model is reconstructed. Figure 6 shows the framework of the improved Kriging-model-based optimization design algorithm.

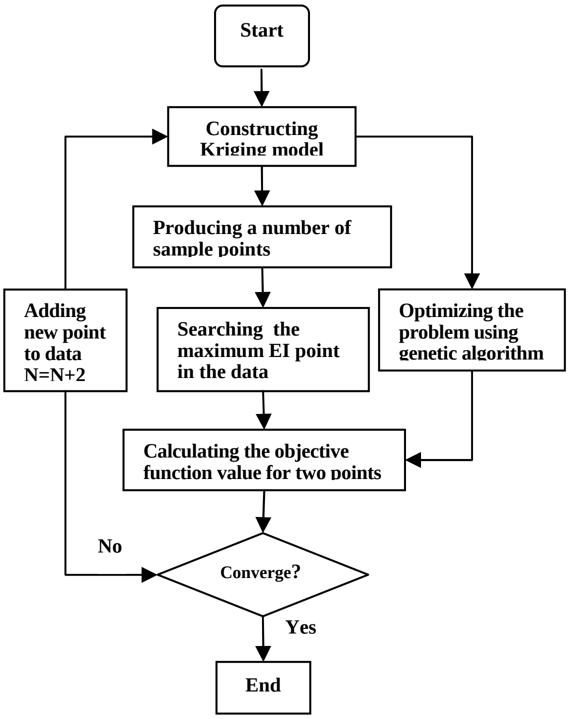


Fig. 6. Framework of the improved Kriging-model-based optimization design algorithm.

6.2 Drag reduction optimization design of RAE2822 airfoil

The Hicks-Henne shape function is adopted to describe the airfoils' geometry perturbation. 10 design variables are chosen with 5 for upper surface and 5 for lower surface of airfoil respectively. 100 initial sample points are selected. The aerodynamic performance of sample airfoils are evaluated by RANS Solver. For the solution of RANS euquations, the central scheme for spatial discretization and a fully implicit time-stepping method are utilized; for turbulence simulation B-L turbulence model is used. Schematics of computational grid of C type for RAE2822 airfoil is showed in the figure 7. The genetic algorithm is applied to searching the optimum point.

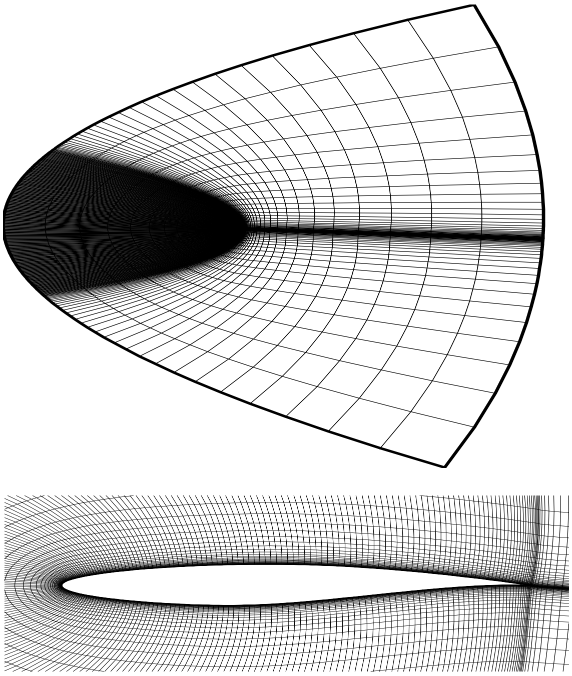


Fig. 7. Schematics of computational grid for RAE2822 airfoil(grid cell：344×96)

The above mentioned improved Kriging-model-based optimization design technique is applied to the drag reduction optimization design for the airfoil. The test problem is minimizing the drag coefficient of an airfoil, at an angle of attack 2.7°, 0.73 freestream Mach number and 6.5×10^6 Reynolds number. The constraints are airfoil's cross-section area and lift coefficient, the baseline airfoil is RAE2822. In mathematical form the constraints can be expressed as follows:

Constraints: (1) $\frac{A}{A_0} - 0.995 \geq 0$

(2) $\frac{C_l}{C_{l0}} \approx 1.0$

Figure 8 and figure 9 show the comparison of pressure and geometry between the optimal and baseline airfoil. It can be seen that the surface pressure distribution of the optimal airfoil is smooth, and shock wave is completely eliminated, the drag coefficient is greatly decreased, that is, aerodynamic performance of the airfoil improved greatly. Table 1 gives lift coefficient, drag coefficient, moment coefficient and cross-section area for baseline airfoil and optimal airfoil. After the optimization design, the drag coefficient is decreased from 0.018767 to 0.012447, i.e. decreased by 33.6%, while the lift coefficient changes less than 1% and the cross-section area of the optimal airfoil is almost the same as the baseline airfoil.

When the number of EI cycle reachs nine in the airfoil optimization process, the convergence criterion is achieved, the number of samples increases from 100 to 118. The surface pressure coefficients of the airfoil in different EI cycle are showed in figure 10. The shock wave on the upper surface of the airfoil weakens gradually with EI cycle increasing, and the optimization result is improved gradually. Figure 11 shows the change of fitting error of Kriging model on EI cycle. It indicates that the accuracy of the Kriging model improved largely with more and more samples added to the sample set, the fitting error is decreased from 10.6% to 0.094%.

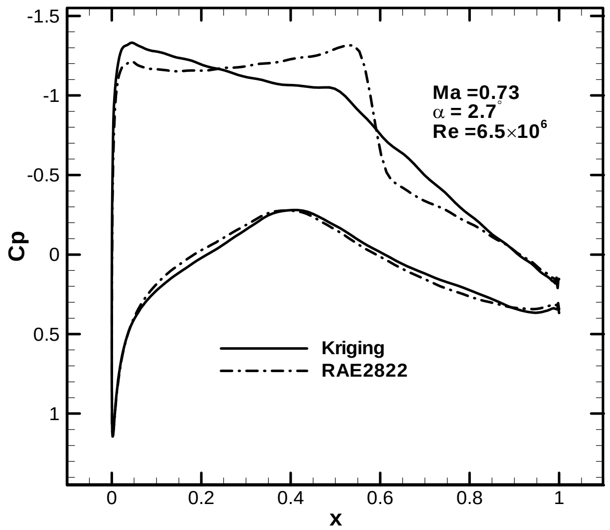


Fig. 8. Comparison of pressure distribution between the optimal and initial airfoil

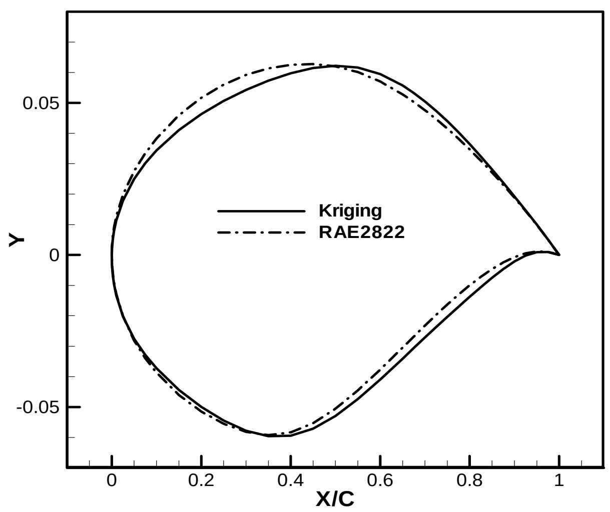


Fig. 9. Comparison of geometry between the optimal and baseline airfoil

Table 1 Optimization results of Kriging model

Parameters	Basis airfoil	Optimum airfoil (Kriging)	Optimum airfoil (N-S)	Change	Error
C_l	0.8650	0.8564	0.8573	0.00088	0.1%
$C_d(\times 10^{-2})$	1.8767	1.2447	1.2459	0.00117	0.094%
C_m	-0.10126	-0.09340	-0.09354	-0.00015	0.16%
A	0.077723	0.077989		0.000266	

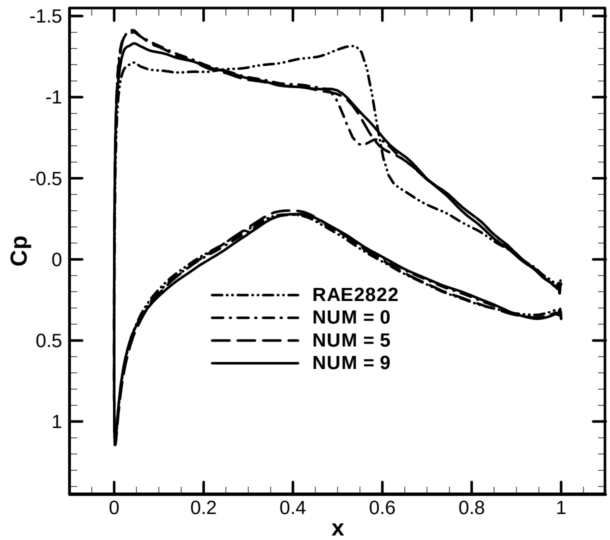


Fig. 10. Comparison of pressure distribution in different EI cycle

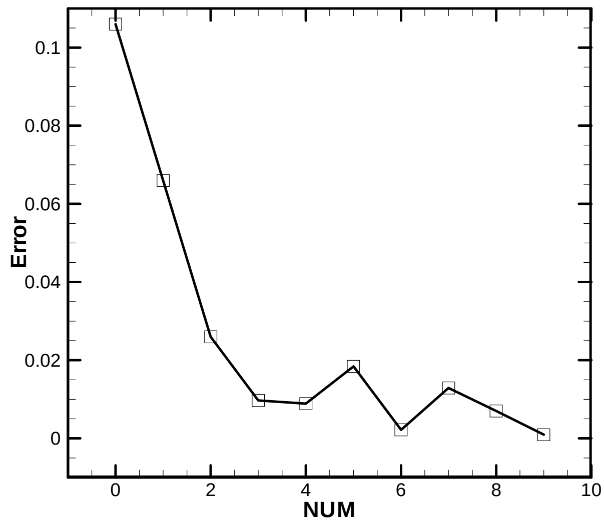


Fig. 11. The change of fitting error of Kriging model on EI cycle

7 Conclusion

With the combination of Latin hypercube sampling, improved Kriging model and genetic optimization algorithm, an improved Kriging-model-based optimization design method is developed. Once the initial samples are formed by Latin hypercube sampling, by simultaneously adding the sample point with maximum EI (Expected Improvement) and the optimal point from the optimization of initial samples, the improved Kriging-model of higher accuracy can be formed gradually, and the final optimization of given objective can be realized with several cycle of addition of the sample point with maximum EI and optimum point of the former samples.

The fitting accuracy of the improved Kriging model is validated through the tests of a one-dimensional function and an aerodynamic problem, which shows that the improved Kriging model can replace the high fidelity CFD analysis solver to accomplish the process of aerodynamic optimization design.

The results of drag reduction optimization design of RAE2822 airfoil indicate that the fitting accuracy of Kriging model can be gradually improved by the method developed in this paper, and aerodynamic performance of the final optimum airfoil can be improved greatly, which shows that the method developed in this paper can be applied to aerodynamic optimization design.

References

[1] Shinkyu J, M.M and K.Y. Efficient optimization design method using Kriging model. AIAA-2004-118.

[2] Mashiro K, Kentaro T, Sinkyu J and Kazuomi Y, Multi-objective Aerodynamic Optimization of Elements' Setting for High-lift Airfoil Using Kriging Model. 44th AIAA Aerospace Sciences Meeting and Exhibit 9-12 January 2006, Reno, Nevada, AIAA-2006-1471 .

[3] Wang Xiaofeng, Xi Guang. Aerodynamic Optimization Design for Airfoil Based on Kriging Model. Acta Aeronouticaet Astronautica Sinica, 2005,26(5)：545-549.

[4] Su Wei, Gao Zhenghong, Xia Lu. An Effective Surrogate-Assisted Genetic Algorithm for Airfoil Aerodynamic Optimization Design. Journal of Northwestern Polytechnical University, 2008， 26(3)：303-307.

[5] Giunta, A. A, Wojtkiewicz Jr, S. F., Eldred, M. S, “Overview of Modern Design of Experiments Methods for Computational Simulations”, AIAA paper 2003-649, 2001.

[6] M Sekishiro, G Venter, V Balabanov. Combined Kriging and Gradient-Based Optimization Method. 11th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference 6-8 September 2006, Portsmouth, Virginia. AIAA 2006-7091.

[7] Zhang Keshi. Multidisciplinary Design Optimization Method and Its Application in Aircraft Design. PhD thesis, Northwestern Polytechnical University.2006

[8] Liu Zhanhe, Song Wenping, Song Bifeng. Study on Multi-Objective Optimization of Airfoil Design with Complex Optimum Method. Journal of Northwestern Polytechnical University, 2004， Vol.22(6)：795-799.

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