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An improved adaptive sampling and experiment design method for aerodynamic optimization

Huang Jiangtao [a,*], **Gao Zhenghong** [b], **Zhou Zhu** [a], **Zhao Ke** [b]

[a] *Computational Aerodynamics Institute, China Aerodynamics Research and Development Center, Mianyang 621000, China*
[b] *National Key Laboratory of Aerodynamic Design and Research, Northwestern Polytechnical University, Xi'an 710072, China*

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Abstract Experiment design method is a key to construct a highly reliable surrogate model for numerical optimization in large-scale project. Within the method, the experimental design criterion directly affects the accuracy of the surrogate model and the optimization efficient. According to the shortcomings of the traditional experimental design, an improved adaptive sampling method is proposed in this paper. The surrogate model is firstly constructed by basic sparse samples. Then the supplementary sampling position is detected according to the specified criteria, which introduces the energy function and curvature sampling criteria based on radial basis function (RBF) network. Sampling detection criteria considers both the uniformity of sample distribution and the description of hypersurface curvature so as to significantly improve the prediction accuracy of the surrogate model with much less samples. For the surrogate model constructed with sparse samples, the sample uniformity is an important factor to the interpolation accuracy in the initial stage of adaptive sampling and surrogate model training. Along with the improvement of uniformity, the curvature description of objective function surface gradually becomes more important. In consideration of these issues, crowdness enhance function and root mean square error (RMSE) feedback function are introduced in *C* criterion expression. Thus, a new sampling method called RMSE and crowdness enhance (RCE) adaptive sampling is established. The validity of RCE adaptive sampling method is studied through typical test function firstly and then the airfoil/wing aerodynamic optimization design problem, which has high-dimensional design space. The results show that RCE adaptive sampling method not only reduces the requirement for the number of samples, but also effectively improves the prediction accuracy of the surrogate model, which has a broad prospects for applications.

* Corresponding author. Tel.: +86 816 2463133.
E-mail address: hjtcyf@163.com (J. Huang).
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1. Introduction

Surrogate model is widely used in the interpolation, numerical optimization and prediction. It is generally acknowledged that experimental design, which is an important branch of statistics, plays a key role in the construction of a credible surrogate model.

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Through reasonable experiment arrangement and statistical analysis, considerable reduction of the number of experiments and improvement of the test quality can be realized. As surrogate model is established based on the sampling data, for a designated surrogate model, reasonable sampling distribution in space has a significant impact on the prediction accuracy because surrogate model is established based on the sampling data, i.e., experimental design of samples is an important research aspect. Random design, orthogonal design, uniform design and Latin hypercube design are the classical experimental design methods, which have been widely used in fluid mechanics and aerodynamics design field. However, traditional experiment design does not consider the object function curvature and has obvious blindness in sampling process, which causes huge cost in improving the prediction accuracy.

With the rapid development of computer, the aerodynamic design goes into numerical optimization design stage from the "Cut and Try" generation so that the numerical optimization becomes primary in modern aircraft design. However, in some aerodynamic optimization problems, such as multi-object design, refined optimization which contains large scale design variables still needs huge workload. So it is quite requisite to establish a reasonable sampling method which can ensure the surrogate model prediction accuracy and reduce the number of samples needed simultaneously. According to calculation amount and prediction accuracy in the aerodynamic design, in this paper, an improved adaptive sampling method is established, both of which can ensure sample space distribution uniformity and describe the curvature of the object function. The improved adaptive sampling method is applied to typical test function, airfoil and wing-body aerodynamic design.

2. An improved adaptive sampling method

In this paper, radial basis function (RBF) is used to build the surrogate model, which is a linear combination of basic functions. The concept was proposed by Buhmann and Fasshauer[1,2] and widely used in many researching domains, such as interpolation, neural network training, data predicting and grid deformation.[3] The interpolation model based on RBF can be expressed as:

$$\mathrm{RBF}(\boldsymbol{x}) = \sum_{i=1}^{N} a_i \phi(\|\boldsymbol{x} - \boldsymbol{x}_i\|) + p(\boldsymbol{x}) \tag{1}$$

where $\phi(\cdot)$ and $\|\cdot\|$ represent the basis function and the Euclidean norm respectively, a_i is RBF coefficient. The polynomial method was selected for $p(\boldsymbol{x})$:

$$p(\boldsymbol{x}) = \beta_0 + \sum_{n=1}^{m} \beta_n x_{i,n} \tag{2}$$

where m is the dimension of radial center vector, and β_n is polynomial coefficient. Then the model can be expressed as a form of matrix:

$$\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{0} \end{bmatrix} = \begin{bmatrix} \boldsymbol{R} & \boldsymbol{F} \\ \boldsymbol{F}^{\mathrm{T}} & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\beta} \\ \boldsymbol{a} \end{bmatrix} \tag{3}$$

where

$$\boldsymbol{R} = \begin{bmatrix} \phi_{1,1} & \phi_{1,2} & \cdots & \phi_{1,n} \\ \phi_{2,1} & \phi_{2,2} & \cdots & \phi_{2,n} \\ \phi_{n,1} & \phi_{n,2} & \cdots & \phi_{n,n} \end{bmatrix}$$

$$\boldsymbol{F} = \begin{bmatrix} f_{1,1} & f_{1,2} & \cdots & f_{1,n} \\ f_{2,1} & f_{2,2} & \cdots & f_{2,n} \\ f_{n,1} & f_{n,2} & \cdots & f_{n,n} \end{bmatrix}$$

where f is the monomial components, $\boldsymbol{y}$ the value vector of evaluation point. The unknown vector of interpolation matrix can be calculated by formulas:

$$\boldsymbol{a} = (\boldsymbol{F}^{\mathrm{T}}\boldsymbol{R}^{-1}\boldsymbol{F})^{-1}\boldsymbol{F}^{\mathrm{T}}\boldsymbol{R}^{-1}\boldsymbol{y} \tag{4}$$

$$\boldsymbol{\beta} = [\boldsymbol{R}^{-1} - \boldsymbol{R}^{-1}\boldsymbol{F}(\boldsymbol{F}^{\mathrm{T}}\boldsymbol{R}^{-1}\boldsymbol{F})^{-1}\boldsymbol{F}^{\mathrm{T}}\boldsymbol{R}^{-1}]\boldsymbol{y} \tag{5}$$

Then, interpolation system based on RBF can be established:

$$\hat{\boldsymbol{y}}(\boldsymbol{X}_*) = \boldsymbol{r}^{\mathrm{T}}\boldsymbol{\beta} + \boldsymbol{f}^{\mathrm{T}}\boldsymbol{a} \tag{6}$$

where $\boldsymbol{X}_*$ is an evaluation point, and $\boldsymbol{r}$ the basis function vectors. The weighted Euclidean distance used in basis function is given by:

$$\|\boldsymbol{X}_* - \boldsymbol{X}\| = \frac{1}{R}\sqrt{\sum_{j=1}^{n} \omega_j^2 (\boldsymbol{X}_{j*} - \boldsymbol{X}_j)^2} \tag{7}$$

where R is the radius of RBF.

In this paper, ω_j are determined by Quantum-Behaved particle swarm optimizer (PSO)[4] and leave-one-out cross-validation (LOOCV) criterion.[5]

Based on the power function and the native space norm, a standard uncertainty measure for RBF interpolation has been constructed by Jakobsson et al.[6] They quantify the component of interpolation error which depends on the basis function and sample locations and can be expressed as:

$$P(\boldsymbol{X}_*) = \sqrt{\phi(0) + (\boldsymbol{F}\boldsymbol{R}^{-1}\boldsymbol{r} - \boldsymbol{f})^{\mathrm{T}}(\boldsymbol{F}^{\mathrm{T}}\boldsymbol{R}^{-1}\boldsymbol{F})^{-1}(\boldsymbol{F}\boldsymbol{R}^{-1}\boldsymbol{r} - \boldsymbol{f}) - \boldsymbol{r}^{\mathrm{T}}\boldsymbol{R}^{-1}\boldsymbol{r}} \tag{8}$$

where $P(\boldsymbol{X}_*)$ is scaled by the native space norm $\|\hat{\boldsymbol{y}}_{\mathrm{s}}\| = \boldsymbol{\beta}^{\mathrm{T}}\boldsymbol{R}\boldsymbol{\beta}$.

The sampling criteria of RBF surrogate model are further carried out, in which curvature features of the target surface function and a sample separation function are used. Hence, they can achieve local refinement and distribution exploration. The local curvature characteristics are realized by Laplace operation and the separation function is implemented through the energy function and the local space norm. In combination of those two aspects, the sampling criteria are defined as follows[7]:

$$C = (|\nabla^2\hat{\boldsymbol{y}}| + \varepsilon)P^2(\boldsymbol{x})\|\hat{\boldsymbol{y}}_{\mathrm{s}}\| \tag{9}$$

where ε is a little parameter to avoid zero value; $\nabla^2\hat{\boldsymbol{y}}$ can be easily calculated by formula[7]:

$$\nabla^2\hat{\boldsymbol{y}} = \frac{\partial^2\boldsymbol{r}^{\mathrm{T}}}{\partial\boldsymbol{x}_i^2}\boldsymbol{\beta} + \frac{\partial^2\boldsymbol{f}^{\mathrm{T}}}{\partial\boldsymbol{x}_i^2}\boldsymbol{a} \tag{10}$$

The maximum values of C indicate the new sample locations and can realize the balance among locations where the data are nonlinear. At the same time, the adding points are in unsampled regions.

The above criterion improves the effectiveness of sample collection greatly. However, for the basic sparse samples, interpolation uncertainty of the model plays a key role in the initial stage of the interpolation model training. With the number of samples increases, accurate description of curvature for