COMPARISON OF INFILL SAMPLING CRITERIA IN KRIGING-BASED AERODYNAMIC OPTIMIZATION

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Keywords: *kriging; infill sampling criteria (ISC); optimization*

Abstract

Kriging-based optimization methods are of great interest for aerodynamic design optimization where high-fidelity thus time-consuming computational fluid dynamics (CFD) are used. In the framework of kriging-based optimization, a core technique called sampling infill criteria (also called adaptive sampling) is used both to search the design space and to refine the surrogate models. Among all the infill criteria, expected improvement (EI) is the favorite one while others are also still in use. However, there is little research compared these criteria when kriging-based optimization method is applied in the aerodynamic design optimization. The following paper addresses this issue by investigating 6 types of infill criteria in the drag minimization problem of the RAE2822 airfoil with different number of design variables. For each infill criterion and each number of design variables, the optimization process is repeated 30 times, and the averaged value and standard deviation are compared. The results show that, some criteria can be comparable to EI or even slight better than EI, while some criteria are much worse.

1 Introduction

While the performance of computing is growing rapidly in the modern world, the demand for more accurate computer simulation towards aircraft design is also growing. Hence, it is still rarely feasible to search a design space directly using expensive computer codes such as high fidelity CFD or CSD codes. The use of surrogate models, then, is of great interest and playing an increasingly important role in the aerodynamic and multidisciplinary design optimization. Among many of the surrogate models, kriging is the most popular one due to its ability to effectively capture the complicated responses and providing an error estimation of the prediction.

In the process of the kriging-based optimization, the global optimum can't be found if we only utilize the kriging models built from initially sampled data, since the models are not accurate globally. Hence, new sample points in the promising regions should be added, then the kriging models can be refined; this process is repeated until the global optimum is found or some stop criteria are met. This process is so-called iterative sampling refinement (or adaptive sampling) and the criteria to sample the promising regions are so-called infill sampling criteria (ISC). Since the iterative strategy represents the one of the key technique of the surrogate-based optimization, the choice of ISC is then of great importance. In the efficient global optimization (EGO) method [1], the expected improvement (EI) infill criterion is introduced and gained extensive attention in the application of the aerodynamic design optimization [2][3]. However, other infill criteria are also available and demonstrated to be effective too. For example, J. Laurenceau [4] used the lower confidence bounding (LCB) in the optimization design of airfoil and wing; F. A. C. Viana [5] used the probability of improvement (PI) to update the kriging model; W. P. Song [6] minimize the surrogate model and maximize the EI simultaneously to update the kriging model in the airfoil design optimization. In spite of this, little research compared these infill criteria when the kriging-based optimization method is applied in the aerodynamic optimization. This paper aims to compare 6 typical ISC [7] involving: minimizing the predictor (MP), lower confidence bounding (LCB), expected improvement (EI), probability of improvement (PI), maximizing the predicted error (ME), and combining EI with MP (EI+MP, two points added at a time), when applied to the constrained drag minimization of the RAE2822 airfoil.

2 Overview of Kriging

Kriging is a statistical interpolation method suggested by Krige [8] in 1951 and mathematically formulated by Matheron [9] in 1963. Kriging was widely used in the context of geostatistical problems. In 1989, kriging was extended by Sacks et al [10] for the design and analysis of deterministic computer experiments. Then it was widely used as a surrogate modeling technique for predicting the output of computer codes in simulation-based analysis and optimization [11][12][13]. The ordinary kriging is used in this paper.

- Kriging Predictor and Mean Squared Error

The kriging treats the output of a deterministic computer experiment as a constant term plus a stochastic process:

$$Y(\mathbf{x}) = \beta_0 + Z(\mathbf{x}) . \qquad (1)$$

The stationary random process $Z(\bullet)$ has mean zero and covariance of

$$Cov[Z(\mathbf{x}), Z(\mathbf{x}')] = \sigma^2 R(\mathbf{x},\mathbf{x}') , \qquad (2)$$

where σ^2 is the process variance of $Z(\bullet)$ (it is assumed that $\sigma^2(\mathbf{x}) \equiv \sigma^2$ for all $\mathbf{x}$, and R is the spatial correlation function that only depends on the Euclidean distance between two sites $\mathbf{x}$ and $\mathbf{x}'$.

We assume that the output of a computer code can be approximated by a linear combination of the observed data $\mathbf{y}_s$, the kriging approximation of $y(\mathbf{x})$ at an untried $\mathbf{x}$ is formally defined as

$$\hat{y}(\mathbf{x}) = \sum_{i=1}^{n_s} w_i y_i = \mathbf{w}^{\mathrm{T}} \mathbf{y}_{\mathrm{S}} , \qquad (3)$$

where $\mathbf{w} = (w^{(1)},...,w^{(n_s)})^{\mathrm{T}}$ are the weight coefficients (called kriging weights). We replace $\mathbf{y}_{\mathrm{S}} = (y^{(1)},...,y^{(n_s)})^{\mathrm{T}}$ with the corresponding random quantities $\mathbf{Y}_{\mathrm{S}} = (Y^{(1)},...,Y^{(n_s)})^{\mathrm{T}}$.

By minimizing the mean squared error (MSE) of this predictor, we can obtain the following kriging predictor

$$\hat{y}(\mathbf{x}) = \hat{\beta}_0 + \mathbf{r}^{\mathrm{T}}(\mathbf{x})\mathbf{R}^{-1}(\mathbf{y}_s - \mathbf{1}\hat{\beta}_0) , \qquad (4)$$

where $\mathbf{1}$ is unit column vector filled with ones and

$$\hat{\beta}_0 = \left(\mathbf{1}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{1}\right)^{-1} \mathbf{1}\mathbf{R}^{-1}\mathbf{y}_{\mathrm{S}} , \qquad (5)$$

and

$$\mathbf{R} := \left[R(\mathbf{x}^{(i)},\mathbf{x}^{(j)})\right]_{ij} \in \mathbb{R}^{n\times n}, \mathbf{r}(\mathbf{x}) := \left[R(\mathbf{x}^{(i)},\mathbf{x})\right]_i \in \mathbb{R}^n . \quad (6)$$

The MSE of the kriging prediction at any untried $\mathbf{x}$ can be proven to be

$$MSE[\hat{y}(\mathbf{x})] = \hat{\sigma}^2[1 - \mathbf{r}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{r} + (1-\mathbf{1}\mathbf{R}^{-1}\mathbf{r})^2 / \mathbf{1}^{\mathrm{T}}\mathbf{R}\mathbf{1}] \quad (7)$$

where

$$\hat{\sigma}^2 = \frac{1}{n_s}(\mathbf{y}_s - \mathbf{1}\hat{\beta}_0)^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{y}_s - \mathbf{1}\hat{\beta}_0). \qquad (8)$$

- Correlation Models

The construction of the correlation matrix $\mathbf{R}$ and the correlation vector $\boldsymbol{r}$ requires the calculation of the correlation functions. The correlation function for random variables at two sites $\mathbf{x}^{(i)},\mathbf{x}^{(j)}$ is assumed to be only dependent on the spatial distance. Here we focus on a family of correlation models that are of the form

$$R(\mathbf{x}^{(i)},\mathbf{x}^{(j)}) = \prod_{k=1}^{n_v} R_k(\theta_k, \mathbf{x}_k^{(i)} - \mathbf{x}_k^{(j)}) . \qquad (9)$$

The correlation function used here is the cubic spline:

$$R_k = \begin{cases} 1 - 15\xi_k^2 + 30\xi_k^3 & \text{for } 0 \le \xi_k \le 0.2 \\ 1.25(1-\xi_k)^3 & \text{for } 0.2 < \xi_k < 1 \\ 0 & \text{for } \xi_k \ge 1 \end{cases} , \qquad (10)$$

where

$$\xi_k = \theta_k \left| \mathbf{x}_k^{(i)} - \mathbf{x}_k^{(j)} \right|. \tag{11}$$

- Kriging Fit

Hyper parameters of kriging, $\boldsymbol{\theta} = (\theta_1, ..., \theta_{n_v})$, can be tuned by solving maximum likelihood estimation (MLE) problem:

$$\text{MLE} = \arg\max_{\boldsymbol{\theta}} \left(-\frac{1}{2} \left[n_s \ln(\hat{\sigma}^2) + \ln|\mathbf{R}| \right] \right). \tag{12}$$

In this paper, the quasi-Newton method is used.

3 Infill Sampling Criteria

There are several kinds of infill criteria for kriging-based optimization [7]. The 6 kind of common used infill criteria and corresponding constraint handling methods in this paper are described in the following, also see [13] for some description.

3.1 Maximizing the Constrained Expected Improvement (EI)

Expected improvement is defined as the improvement we expect to achieve at an untried site $\mathbf{x}$. Assume the random variable $Y \sim N[\hat{y}(\mathbf{x}), s^2(\mathbf{x})]$, where $\hat{y}$ is the kriging predictor defined in Eq.(4), s^2 is mean squared error defined in Eq.(7). Let $y_{\min}$ is the current best objective function value; the improvement is $I = y_{\min} - Y(\mathbf{x}) > 0$. The expected improvement is given by

$$E[I(\mathbf{x})] = \begin{cases} (y_{\min} - \hat{y}(\mathbf{x}))\Phi\left(\dfrac{y_{\min} - \hat{y}(\mathbf{x})}{s(\mathbf{x})}\right) & \\ + s \times \phi\left(\dfrac{y_{\min} - \hat{y}(\mathbf{x})}{s(\mathbf{x})}\right) & \text{if } s>0 \\ 0 & \text{if } s=0 \end{cases}, \tag{13}$$

where $\Phi(\bullet)$ and $\phi(\bullet)$ are the cumulative distribution function and probability density function of standard normal distribution, respectively.

Assume we have a constraint $g(\mathbf{x}) > g_{\min}$, and we also constructed a kriging model for $g(\mathbf{x})$. Following the same logic of the expected improvement, we assume the random variable $G \sim N[\hat{g}(\mathbf{x}), s^2(\mathbf{x})]$. Then, the probability that the constraint is fulfilled is as following:

$$P[G > g_{\min}] = \Phi\left(\frac{g_{\min} - \hat{g}(\mathbf{x})}{s(\mathbf{x})}\right), \tag{14}$$

where s is the root mean square error of the kriging model of the constraint. Then, the constrained expected improvement is:

$$E_c[I(\mathbf{x})] = E\left[I(x) \cap G > g_{\min}\right] = E[I(\mathbf{x})] \bullet P\left[G > g_{\min}\right]. \tag{15}$$

For multiple constraints, the constrained expected improvement is obtained by multiplying each probability that the constraints fulfilled.

3.2 Minimizing the Predicted Objective Function (MP)

This criterion assumes that the surrogate model is globally accurate and we only need to validate the optimum of the surrogate. The optimum point on the surrogate is found and observed to refine the kriging model.

$$\begin{array}{lll} \mathit{Minimize}: & \hat{y}(\mathbf{x}) & \\ s.t. & \hat{g}_i(\mathbf{x}) > 0, & i = 1, \cdots, N_G \end{array}, \tag{16}$$

where N_G is the number of the constraints. The constraints are handled by the optimization algorithm itself, here, the genetic algorithm [11] is used.

3.3 Minimizing the Lower Confidence Bounding (LCB)

The lower confidence bounding is defined as following:

$$LCB(\mathbf{x}) = \hat{y}(\mathbf{x}) - A \times \hat{s}(\mathbf{x}) \quad , \tag{17}$$

where A is a parameter defined by the user, and in this paper, we use 4. In each iteration, we fit the kriging models, and find the lower confidence bounding with constraints:

$$\mathit{Minimize}: \ \text{LCB}_c(\mathbf{x}) = \hat{y}(\mathbf{x}) - A \times s(\mathbf{x}) + \sum_{i=1}^{N_G} \omega_i \left\langle \hat{g}_i(\mathbf{x}) \right\rangle, \tag{18}$$

where $\langle \ \rangle$ denotes the absolute value of the operand if the operand is negative, and returns a value zero otherwise, ω_i is the weight coefficient.

3.4 Maximizing the Probability of Improvement (PI)

The probability of improvement is as following:

$$P\left[I(\mathbf{x})\right]=\Phi\left(\frac{y_{\min}-\hat{y}(\mathbf{x})}{s(\mathbf{x})}\right) \quad . \tag{19}$$

The constraint handed with the same method in the EI criterion, that is, the following optimization problem is executed:

$$maxmize: \ \Phi\left(\frac{y_{\min}-\hat{y}(\mathbf{x})}{s(\mathbf{x})}\right)\times\prod_{i=1}^{N_G}P_i\left[G_i>g_{i,\min}\right] \tag{20}$$

3.5 Maximizing the Mean Squared Error (ME)

As we know, the accuracy of kriging model affects the search of the design space. Since kriging model provides a mean squared error, the global accuracy of the model can be improved by infilling the point whose mean squared error is the maximum in the design space. For constraint handling, the method introduced in EI criterion is also used here, that is

$$maximize: \ s^2\times\prod_{i=1}^{N_G}P_i\left[G_i>g_{i,\min}\right] . \tag{21}$$

3.6 Minimizing the Predicted Objective Function (MP) and Maximizing the Constrained Expected Improvement (EI)

This criterion use EI and MP simultaneously, that is 2 points are founded and added at each iteration cycle.

4 Framework of the Kriging-Based Optimization Method

In this research, a kriging-based optimization system is used [15]. First, several initial sample points are generated in the design space using design of experiments (DoE). Here, we use the Latin hypercube sampling (LHS) [16]; then the samples are observed with parallel computing to save total wall clock time; after that, the kriging models are constructed both for the objective function and the constraints, then the kriging models are refined repetitively by infilling new points obtained with GA under specified infill criteria; this iteration terminates until some stop criteria meet, for instance, the function evaluation budgets exceeds some specified value. The framework of the optimization is shown in Fig. 1.

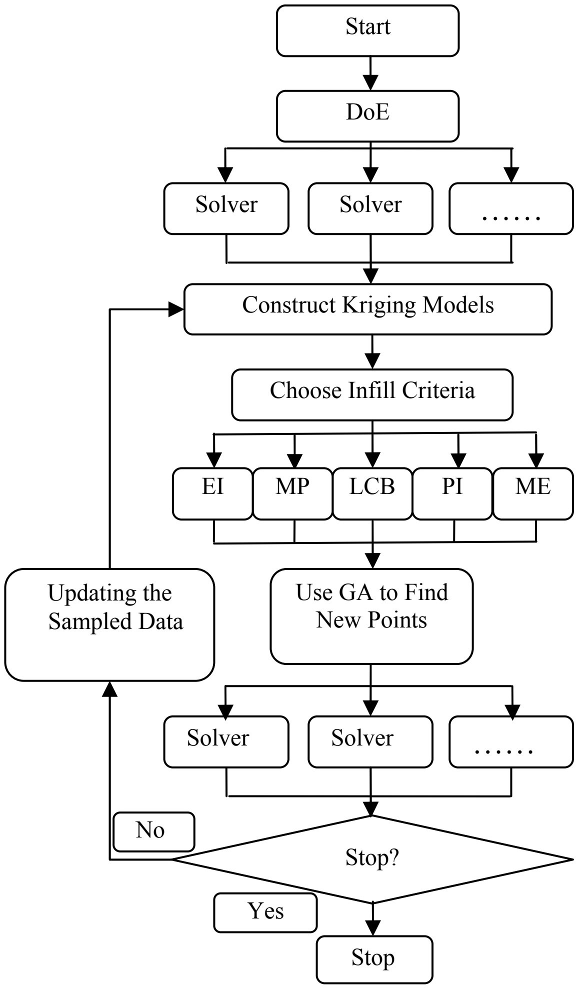


Fig. 1. Framework of the kriging-based optimization method

5 Results

5.1 Validation of Methodology

In general optimization problems, there exist some constraints. To validate the 6 infill criteria and their capability of constraint handling, here we introduce the modified Branin function [17]:

$$f(\mathbf{x}) = (15x_2 - \frac{5.1}{4\pi^2}\times(15x_1-5)^2 + \frac{5}{\pi}\times(15x_1-5)-6)^2$$
$$+10\times((1-\frac{1}{8\pi})\times\cos(15x_1-5)+1)+5x_1 \quad , \quad x_1,x_2=[0,1].$$
$$s.t. \quad g(\mathbf{x}) = x_1x_2 > 0.2. \tag{22}$$

The global optimum and its function value is $(x_1^*,x_2^*)=(0.96773,0.20667), f(x_1^*,x_2^*)=5.5757$. Fig. 2 shows the contour of this function; note that, above the red line is the feasible region.

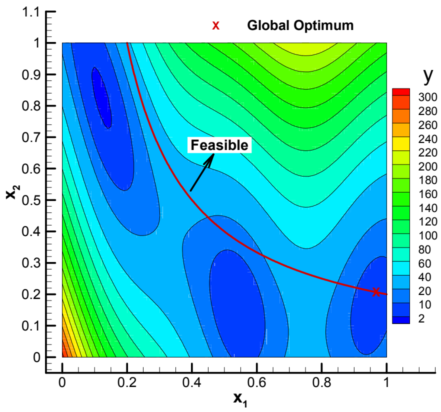
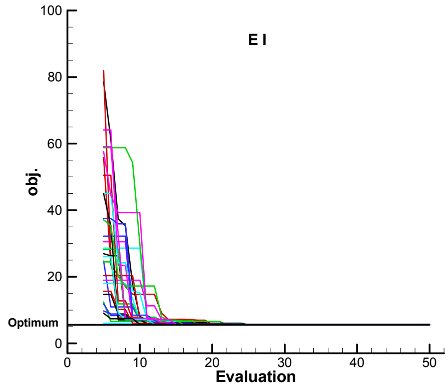


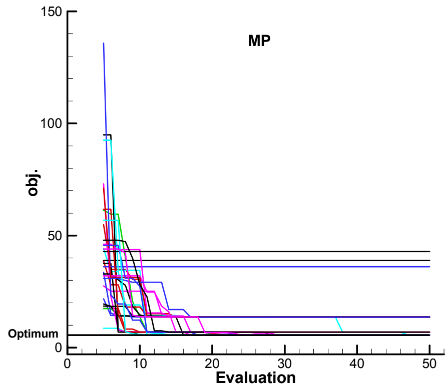
Fig. 2. Contour of the modified Branin function

In each optimization process, 4 initial sample points are generated using LHS, and a total of 50 function evaluation budges are used. For each infill criterion, the entire optimization process is repeated 30 times using LHS from different random-number seed to prevents the “getting lucky” scenario whereby a point in the initial DOE falls on or near the global optimum [18].

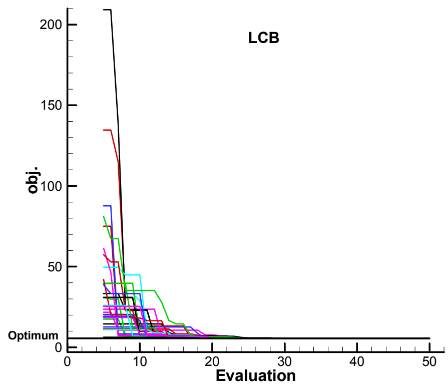
Fig. 3 gives all the 30 convergence histories for each infill criteria. This figure shows that, for EI, LCB, PI, EI+MP, the global optimum is found almost every time. This lies in the balance of exploitation (sampling where it is minimized) and exploration (sampling where the prediction error may be high) for these infill criteria. However, for MP, the global optimum can’t be found every time, since it is a pure exploitation infill criterion, and may be trapped in local optimum if the initial DOE is not “lucky”. The results are similar to MP for ME, since it is pure exploration.



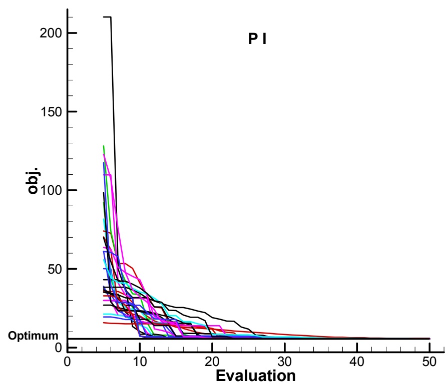
a) Convergence histories for EI infill criterion



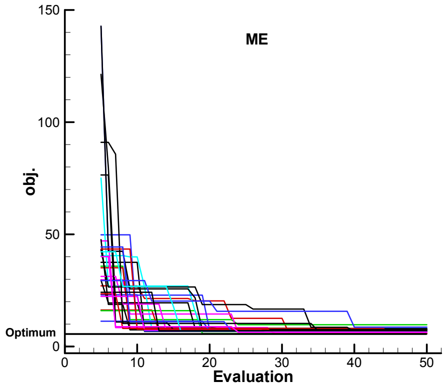
b) Convergence histories for MP infill criterion



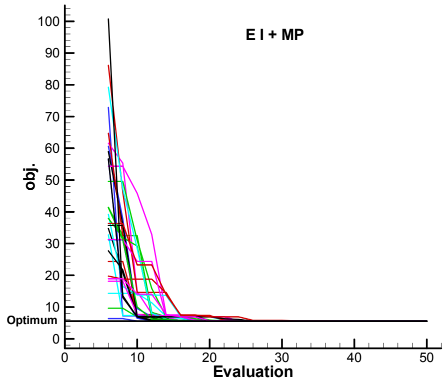
c) Convergence histories for LCB infill criterion



d) Convergence histories for PI infill criterion



e) Convergence histories for ME infill criterion



f) Convergence histories for EI+MP infill criterion

Fig. 3 Convergence histories of the objective for each infill criteria

5.2 Airfoil Design Optimization

The airfoil design optimization problem investigated in this paper is the drag minimization of the RAE2822 airfoil at an angle of attack of 2 deg., Mach 0.73, with three constraints: the airfoil's lift coefficient does not decrease, the absolute value of moment coefficient does not increase, and the maximum thickness of the airfoil dose not decreases. The mathematic model is as following:

$$\begin{array}{lll} \text{design point: } Ma=0.73,\ \alpha=2.0^\circ & & \\ objective: & minimize \quad C_d & \\ s.t. & (1)\ C_l \geq C_{l0} & \\ & (2)\ |C_m| \leq |C_{m0}| & \\ & (3)\ \text{Thickness} \geq \text{Thickness}_0 & \end{array} . \quad (23)$$

The flow analyses are performed with the two dimensional Euler solver on O-typed structured mesh, using the cell-centered finite volume approach. And the second-order Jameson's central scheme is used as spatial scheme. To deform the shape of the airfoil, Kulfan's CST [19] parameterization method is used here.

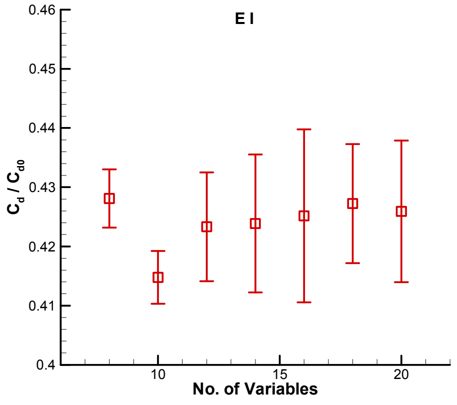
In each optimization process, 2 times of the design variable is taken as the number of initial sample points, and 10 times of the design variable is taken as the number of CFD evaluation budges. For each infill criterion, the entire optimization process is repeated 30 times using LHS from different random-number seed. These optimization processes are carried out for 7 different design variable (8, 10, 12, 14, 16, 18, 20) problems, hence results in a total of 1260 optimization processes.

The mean objective function value for each infill criterion, along with the standard deviation of the objective function is plotted in Fig. 4. The averaged results for each infill criterion are plotted together in Fig. 5 for ease of comparison.

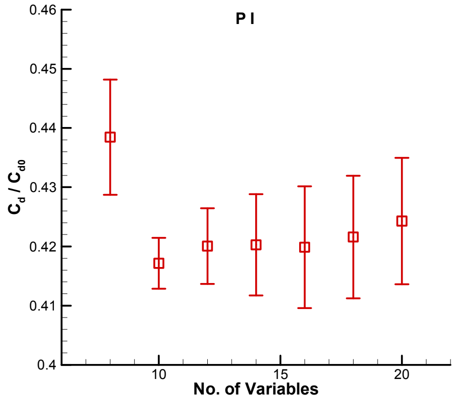
First, we see that, the averaged drag decreased more than a half for all the ISC except ME. Second, the best results are get when the number of variables is 10 for all the infill criteria except ME, and when the dimensionality increases, the results is adversely affected. From Fig. 5 we see that, there are only slight differences among all the ISC except ME and the differences between each other are less than 2% of the baseline's objective function. But if we examine more carefully, we will find that, MP is slightly better than the others, followed by EI+MP and PI, and then EI, LCB. This is somewhat different with the results of analytical function. Finally, ME performs much worse than the others as we expected since it just fill the gap between the sampled points.

Fig. 6 shows the convergence histories for all the ISC when the number of design variable is 10. We can also see that, for ME, not only the averaged objective function is worse, but also the standard deviation is larger than the others. The averaged objective function, standard deviation, and the convergent rate are comparable for all the ISC except ME.

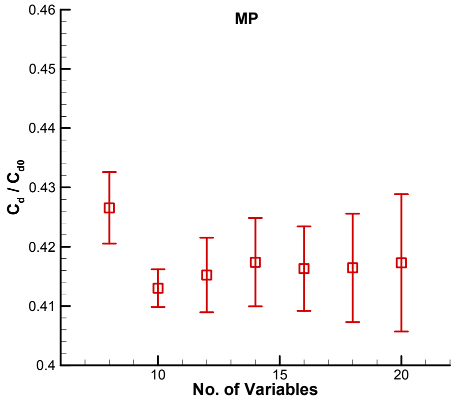
Fig. 7 gives one of the airfoil optimization results including the pressure coefficient distribution and the geometry.



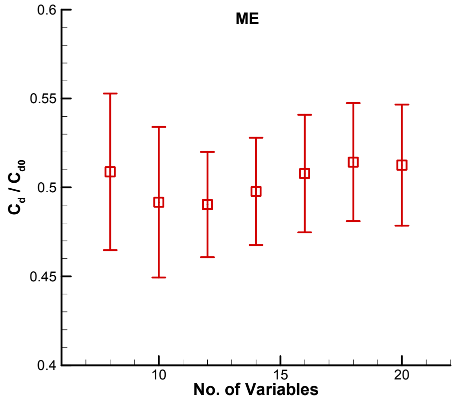
a) EI



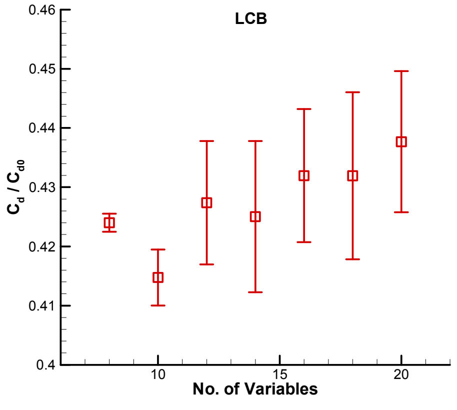
d) PI



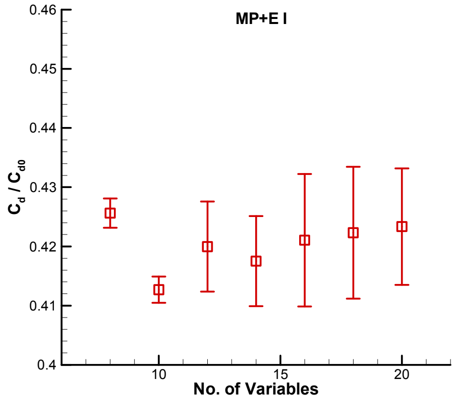
b) MP



e) ME



c) LCB



f) MP+EI

Fig. 4. Averaged results and standard deviation of the optimization design

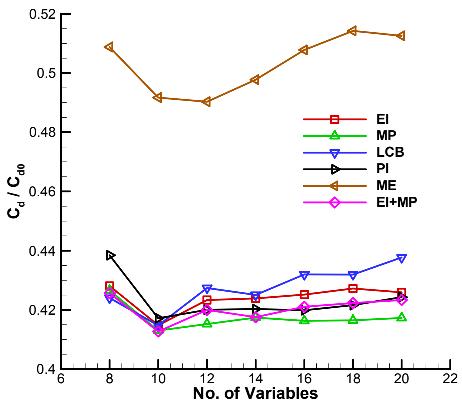
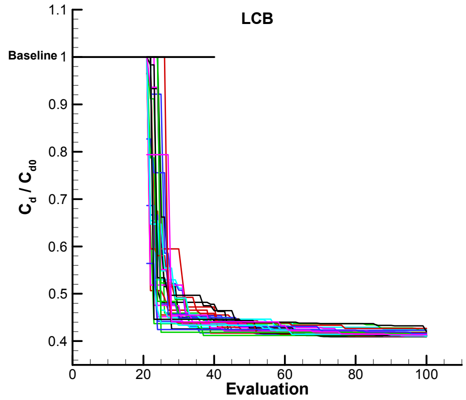
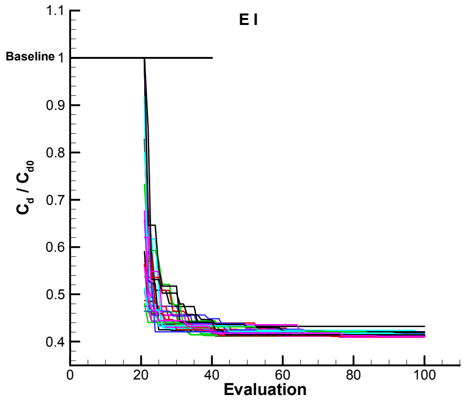


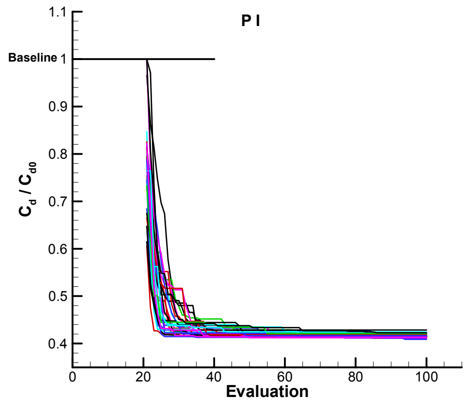
Fig. 5. Averaged results for the 6 infill criteria



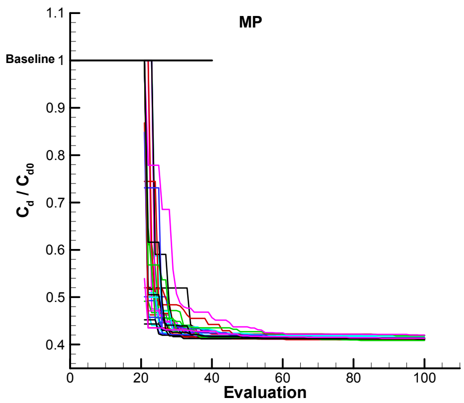
c) LCB



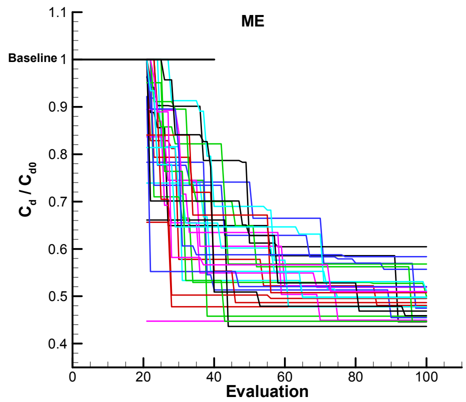
a) EI



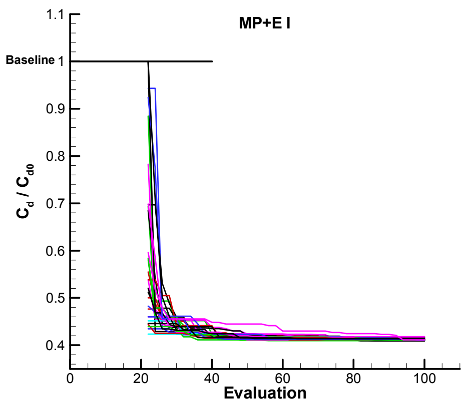
d) PI



b) MP

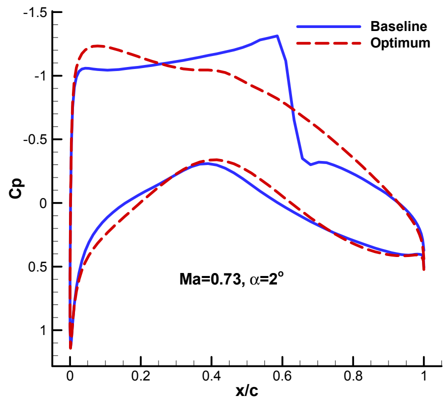


e) ME

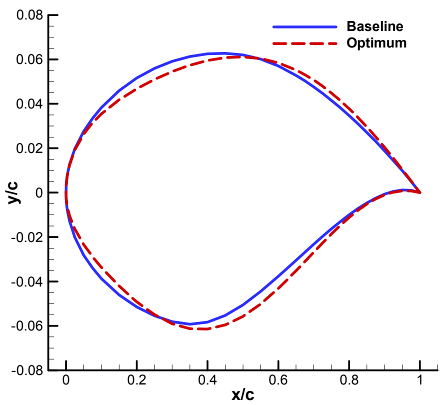


f) MP+EI

Fig. 6. Convergence histories of the objective for each infill criterion of the 10 variable optimization



a) Comparison of the pressure coefficient distributions of the optimized and baseline airfoils



b) Comparison of the geometries of optimized and baseline airfoils

Fig. 7. One of the airfoil optimization results

6 Conclusions and Discussion

The airfoil shape optimization design is introduced to compare the infill sampling criteria in the kriging-based optimization method. To increase the confidence of the statistical analysis, 30 optimizations are carried out for the each problem, and the averaged value and standard deviation are considered. The results show that, for EI, MP, LCB, PI, and EI+MP, they all perform well and there are only slight differences among them, about less than 2 percent of the baseline's objective function. Unexpectedly, MP performs best for the above 5 ISC. And as we expected, ME performs worst.

We can expect that, different ISC can be used simultaneously, that is, several points added at a time and running the simulations in parallel will be more efficient.

7 Acknowledgments

This research is sponsored by the National Natural Science Foundation of China (NSFC) under grant No. 10902088 and the Aeronautical Science Foundation under grant No. 2011ZA53008.

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