Comparison of parallel infill sampling criteria for optimization problems

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Abstract: The efficient global optimization (EGO) algorithm based on the Kriging surrogate model is popular. One of the main problems is to determine the infill sampling criteria. An adaptive distance function is proposed and applied to the EI, PI, and MP criteria. The criteria base on a fix distance is also investigated. Seven test problems were used to evaluate these criteria. The results show that the MMP criterion has poor global search ability. PEI, KB and DMP criteria perform better and have better convergence speed and stability.

1. Introduction
In engineering design, it often involves optimization problems. The objective function values and constraints are mainly obtained by numerical simulation or experiment. Although the population based algorithm (genetic algorithm, particle swarm algorithm, etc.) can get a reliable optimal solution, thousands of population evaluations require a lot of computational time or experimental cost. The surrogate model can replace the expensive calculation. Among many alternative models, Kriging is one of the most popular models[1, 2]. Its main advantage is not only to provide the numerical response of the sample but also to provide the estimation error, which provides a reference for improving the accuracy of the surrogate model.

The efficient global optimization (EGO) algorithm[3] is one of the most successful surrogate-based optimization methods. The surrogate model constructed with initial samples are often not directly used for optimization. Because the initial model is not accurate globally. Therefore, it is necessary to add the sample points to improve the model. Conventional single-point infill sampling criteria include EI, MP, PI, MES (maximizing the predicted error), and LCB (lower confidence bounding) criteria[4, 5]. Parallel infill sampling criteria can be divided into three categories based on how many optimizations and how many criteria are used to generate candidate points at each cycle. The first is to generate multiple sample points in each cycle using one criterion. Ginsbourger et al. [6] derived the q-point expected improvement criterion. However, when the dimension of test problem is greater than two, there is no analytical solution. It needs to be solved by the Monte-Carlo method. Soberster et al.[7] proposed a method for selecting multiple local maximum points of EI. Feng et al.[8] divided the EI into two parts and use the multi-objective optimization algorithm to obtain Pareto solutions of the two parts. The same approach is applied to the weight EI and generalized EI criteria[9]. The above method's main disadvantage is the number of candidate points is uncertain. Correspondingly, many methods have been produced to control the number.

The second is to perform multiple optimizations in each cycle using one criterion. The most typical method is Kriging Believer (KB) developed by Ginsbourger [6]. First, the first candidate point is
selected by standard EI criterion, a ‘fake’ value is selected to update the sample data and the Kriging model. Then the updated model is used to find the next maximum EI point. The ‘fake’ value is mainly using the Kriging prediction value or a constant value. Introducing ‘fake’ value reduces the time for the true function value evaluation. The basal principle is that the EI value near the current point will be reduced by adding a ‘false’ value. Then the next EI extreme point can be found by optimization. Viana et al [10]directly introduces a fixed distance to reduce the EI value near the candidate solution. Similarly, Zhan et al. [11] introduced an influence function to update points. This criterion is called pseudo expected improvement (PEI).

The third is to use multiple single points criteria [12] or surrogate model [13]. The drawbacks are the number of candidate points is limited and it is easy to generate duplicate points. Moreover, multiple single point criteria can be selected for multi-objective optimization[14]. The problem of selecting points is accompanied.

It can be found the second category criterion is simple to implement and can control the number of candidate points. In this paper, first, Zhan's [11] method is introduced into the PI and MP criteria. An adaptive distance function is proposed to produce multiple updating points. Several parallel criteria were compared using the test problem.

2. Efficient global optimization algorithm

2.1. Kriging model
The Kriging model treats the target function as a combination of a regression model and a stochastic process. The regression model is usually treated as a constant. The initial samples are \( S = \{x^1, x^2, K, x^n\}^T \), the corresponding function values are \( y = \{y^1(x), y^2(x), K, y^n(x)\}^T \).

\[
y(x) = \mu + z(x)
\]  

(1)

Where \( \mu \) is a constant, \( z(x) \) is the stochastic process assumed to have mean zero and covariance

\[
\text{cov}(z(x), z(v)) = \sigma^2 R(x, v, \theta)
\]

(2)

between \( z(x) \) and \( z(v) \), where \( \sigma^2 \) is the process variance of the response and \( R(x, v, \theta) \) is the correlation model with parameters \( \theta \). The correlation model is a function of the distance between the sample points. When the distance between the two points is small, the value of the correlation function is near one. As the distance increases, the value tends to zero.

The detail description can be found in [1]. The Kriging predictor and the mean squared error can be obtained as following.

\[
\hat{y}(x) = \mu + r(x)^T R^{-1} (Y - 1\mu)
\]

(3)

\[
\hat{\delta}(x) = \sigma^2 \left( 1 + r^T R^{-1} r + (F^T R^{-1} r - f)^T (F^T R^{-1} F) (F^T R^{-1} r - f) \right)
\]

(4)

2.2. Minimizing the prediction criterion
The premise of applying this criterion is that the surrogate model is sufficiently accurate. This criterion directly searches for the minimum objective based on the surrogate models. But it easy to lead the optimization procedure to trap into a local optimum. In this paper, the criterion is defined as the difference between the current maximum value and the predicted value.

\[
MP = \begin{cases} 
  y_{\text{max}} - \hat{y}(x), & \text{if } y_{\text{max}} - \hat{y}(x) > 0 \\
  0, & \text{if } y_{\text{max}} - \hat{y}(x) < 0 
\end{cases}
\]

(5)
3. Numerical experiments

3.1. Demonstrative example
The Forrester function[15] is used to demonstrate the process of selecting point. The initial sampling points are \( X = [0, 0.5, 0.7, 1] \). Four candidate points are given in each cycle for the parallel criteria. Four cycles are demonstrated for the standard single point criteria. Fig. 1 shows the algorithm based on the EI criterion. The updating point position of PEI, DEI and MEI criteria is close with the standard EI criteria. The difference is the order of adding point. For the KB criterion, the decay of the EI value is rapid because of the change of the hyper-parameter after introducing the ‘fake’ point. The other three only construct Kriging model once, so the EI function is real. The parallel process essentially looks for other local optimal values. DEI and MEI criteria are similar in the first cycle, but the distance function will change with the update of Kriging model for DEI. Fig. 2 shows the algorithm based on the PI criterion. The change in PI function is similar to EI, and the conclusions are the same.

Fig. 1 KB, PEI, DEI and MEI algorithm on Forrester function compared with the standard EI algorithm

Fig. 2 MPI, PPI and DPI algorithm on Forrester function compared with the standard EI algorithm
Fig. 3 MMP, PMP, DMP algorithm on Forrester function compared with the standard EI

Fig. 3 shows the algorithm based on the MP criterion. The standard MP criterion has poor global search ability. Therefore, the candidate points are concentrated near the current optimal value. After the parallel criteria are introduced, the points near the candidate points cannot be added so that the search expands outward. It is conducive to finding local optimal values and improving the global search ability.

3.2. Test problems

Seven test problems are used for this experiment and described below:

Branin function with $n_{\text{dim}} = 2$:

$$f = \left( x_2 - \frac{5}{4\pi} x_1 - 6 \right)^2 + 10 \left( 1 - \frac{1}{8\pi} \right) \cos(x_1) + 10, x_1 \in [-5,10], x_2 \in [0,15]$$  
(6)

Sasena function with $n_{\text{dim}} = 2$:

$$f = 2 + 0.01 \left( x_2 - x_1^2 \right)^2 + \left( 1 - x_1 \right)^2 \left( 2 - x_1 \right) + 7 \sin(0.5x_1) \sin(0.7x_1x_2), x_{1,2} \in [0,5]$$  
(7)

StyblinskiTang7 with $n_{\text{dim}} = 7$:

$$f = \frac{1}{2} \sum_{i=1}^{7} \left( x_i^4 - 16x_i^3 + 5x_i \right), x_i \in [-5,5], i = 1,2,...,7$$  
(8)

Rosenbrock10 with $n_{\text{dim}} = 10$:

$$f = \sum_{i=1}^{9} \left[ 100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2 \right], x_i \in [-2,2], i = 1,2,...,10$$  
(9)

Rastrigin12 with $n_{\text{dim}} = 12$:

$$f = 120 + \sum_{i=1}^{12} \left[ x_i^2 - 10 \cos(2\pi x_i) \right], x_i \in [-1,3], i = 1,2,...,12$$  
(10)

4. Application in inverse design of airfoil

4.1. Test problems

In this paper, the difference between the pressure distribution of the designed airfoil and the target pressure distribution is taken as the objective function, and the inverse design problem is transformed
into the optimization problem.

$$Obj_i = \sum_{i=1}^{N} (C_{\rho}^i - \hat{C}_{\rho}^i)^2$$  \hspace{1cm} (11)

Where the $C_{\rho}$ is the pressure coefficient of the target airfoil, and $\hat{C}_{\rho}$ is the pressure coefficient of the designed airfoil. $N$ is the number of points on the airfoil surface.

The inverse design of the airfoil is performed using the CST method[17-19]. We first give a “thick” shape and a “thin” shape, and then fit the two shapes by CST. We consider the CST parameters of the “thin” shape as the lower bound of the design variables and the parameters of the “thick” shape as the upper bound. The target airfoil should be included in the design space. The design space is shown in Fig. 4. The fourth-order CST method is used, and the total number of variables are 10. It can be seen from the Fig. that the RAE2822 airfoil can be reproduced.

5. Conclusion:
This work extends and compares several parallel infill sampling criteria. Seven test problems are used to test their effectiveness. Test results of different test functions are different. We choose some of the better criteria for the inverse design of a two-dimensional airfoil.

For the low-dimensional test problems, although the MMP criterion is faster, it is easy to trap into the local optimal solution. As the number of updating points increases, the optimization speed of the PMP criterion is not significantly improved. Other criteria have better global search ability. As the number of updating points increases, the optimization rate increases. The DMP and PEI criteria are the most efficient and robust. For the high-dimensional test problems, the DMP criterion performs best. The test results of the DEI, PEI, KB, DPI, PPI and MPI are close. MMP and PMP still have the problem of trapping into the local optimal solution.

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