A KRIGING-BASED UNCONSTRAINED GLOBAL OPTIMIZATION ALGORITHM

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Abstract: Efficient Global Optimization (EGO) algorithm with Kriging model is stable and effective for an expensive black-box function. However, How to get a more global optimal point on the basis of surrogates has been concerned in simulation-based design optimization. In order to better solve a black-box unconstrained optimization problem, this paper introduces a new EGO method named improved generalized EGO (IGEGO), in which two targets will be achieved: using Kriging surrogate model and guiding the optimal searching direction into more promising regions. Kriging modeling which can fast construct an approximation model is the premise of performing optimization. Next, a new infill sampling criterion (ISC) called improved generalized expected improvement which round off Euclidean norm on variation of the optimal solutions of parameter θ to replace parameter g can effectively balance global and local search in IGEGO method. Twelve numerical tests and an engineering example are given to illustrate the reliability, applicability and effectiveness of the present method.

Index terms: Global optimization, Black-box function, Efficient Global Optimization (EGO), Kriging model, Infill sampling criterion.
I. INTRODUCTION

Today’s engineering and structural problems including parametric experiments design, real-time simulation and hardware in the loop are computationally expensive and limit space search and optimization of design problems. Utilizing optimization to directly evaluate expensive computer simulation is a quite time-consuming process. To avoid this situation, surrogate models or meta-models can be cheaply constructed and appropriately applied to optimization. It is becoming widely used in many engineering optimization fields. This is called approximation optimization. Comparing with traditional response surface method, Kriging model [1, 2] which can provide an exact interpolation and minimize the error estimates in the spatial distribution is one of the widely used global approximation model [3]. In addition, Global optimization methods have been extensively applied to a large number of simulation optimization problems. Efficient Global Optimization (EGO) method developed by Jones et al. [4] first fits a Kriging model by a set of initial sampling points obtained by Latin Hypercube designs (LHD) and function evaluations. After that, infill sampling criterion Maximizing expected improvement (EI) is used to find next optimum which often has a minimum function value and a maximum instability.

For EGO method, M. Kanazaki et al. [5] developed mixed-fidelity efficient global optimization using Kriging model and applied to design of supersonic wing. Concurrent efficient global optimization algorithm presented by B. Horowitz et al. [6] was applied to a parallel optimization problem on polymer injection strategies. A novel methodology, based on Kriging and expected improvement, was proposed by S.U. Rehman et al. [7] and was applied to robust unconstrained optimization problems. J. M. Parr et al. [8] introduced an improved EGO method which selects multiple updates based on Pareto optimal solutions to show improvement over a number of existing methods. S. Sakata et al. [9] proposed a structural optimization method using Kriging approximation.

Furthermore, function evaluations should be strictly limited so as to enhance optimal efficiency as soon as possible with the appearance of more complex and expensive computer simulations or black-box function. What’s more, an applicable and efficient infill sampling criterion need be found to realize a further improvement. D. Jones [10] presented seven ISCs to obtain next optimal sampling point for global or local optimization. A multi-objective ISC is devised to enhance EGO performances by S. Yi et al. [11]. D. Huang et al. [12] used an augmented
expected improvement function to extend the efficient global optimization. A. Chaudhuri et al. [13] proposed an adaptive target setting method to adding multiple points in each EGO cycle. For generalized expected improvement, Schonlau, M. Et al.[14] derived a generalized expected-improvement criterion that allows control of how global the search is and describe the relative stopping rule. Several infill sampling criteria is proposed by M. J. Sasena et al. [15] to reduce the metamodel error and influence how locally or globally EGO searches. A novel approach –the clustered multiple generalized expected improvement for surrogate models is present by W. Ponweiser et al. [16] to perform a sensitive balancing between the global and local explorative search behavior.

However, it is necessary for researchers to find a global optimum or a ‘well-behaved’ point by using the least function evaluations and improper ISC. This paper, therefore, introduces a new EGO method called improved generalized EGO (IGEGO), in which two targets need be realized. One is using Krigeing modeling method to construct approximation model. The other is employing the improved ISC to guide the global optimal exploration direction into a more promising region. The two parts will be discussed in detail in the following sections.

The paper structure can be stated as following: Krigeing model in global optimization is given in Section 2. Next, GEGO method is simply described in Section 3. Furthermore, the proposed IGEGO method which can ensure the stability and effectiveness of obtaining global optimal point is shown in detail in Section 4. Additionally, twelve numerical tests and an engineering application are used to discuss and analyze the feasibility and effectiveness of IGEGO in Section 5. Finally, conclusions are given in Section 6.

II. Kriging Model

Kriging model is a combination of a polynomial model with a linear regression of the data plus random process with realization of a normally distributed Gaussian random process [17]:

\[
\hat{y}(x) = \sum_{j=1}^{p} \beta_j f_j(x) + z(x)
\]

where \( X = [x_1, \ldots, x_m] \) with \( x_i \in \mathbb{R}^n \) and responses \( Y = [y_1, \ldots, y_m] \) with \( y_i \in \mathbb{R}^q \) are design sites, \( \hat{y}(x) \) is the unknown function of interest, regression function \( f(x) \) composed with primary functions is a known polynomial function of \( x \). The covariance matrix of is given by

\[
\text{Cov}[z(x_i), z(x_j)] = \sigma^2 R[\Theta, x_i, x_j],
\]
where process variance

\[ \sigma^2 = \frac{1}{m}(Y - F\hat{\beta})^T R^{-1}(Y - F\hat{\beta}) \]  

is maximum likelihood estimate (MLE) of the variance for \( z(x) \), \( R \) is a symmetric and positive definite coefficient matrix obtained by Gaussian correlation function \( (R(\theta) = \exp(-\theta | x - x_i |^2) ) \) in engineering practice. Parameter \( \theta \) controls the range of influence on nearby points, will directly affect the accuracy of the Kriging model. For Gaussian process, the optimal parameter \( \theta \) is obtained by

\[
\min \{\psi(\theta) = \sigma^2 | R | \}\{m\}.
\]  

Finally, the best linear unbiased predictor \( \hat{y}(x) \) can be given by

\[ \hat{y}(x) = f(x)^T \hat{\beta} + r(x)^T \hat{\gamma}, \]  

where \( \hat{y} = R^{-1}(Y - F\hat{\beta}) \) and \( r(x)^T = [R(\theta, x, x_1), \ldots, R(\theta, x, x_m)] \), furthermore, the least squares estimate of undetermined regression coefficient \( \hat{\beta} \) is given by

\[ \hat{\beta} = (F^T R^{-1} F)^{-1} F^T R^{-1} Y. \]  

III. GENERALIZED EGO METHOD

i. EGO method

EGO method firstly takes an initial, small data sample within the design space and fits a Kriging approximation model. Next, the EI-based infill sampling criterion (ISC) simultaneously considering the estimated function value and the standard error is used to obtain the next optimal point. The above process is looped until the stopping criteria are met. In this procedure, the handling of EI plays an important role in EGO method. The expected improvement (EI) is defined by

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

Where, \( f_{\text{min}} \) is the true minimum objective function value searched so far, \( \hat{y} \) is the estimated objective function obtained by Kriging model, \( s \) is the standard error, \( \phi(\cdot) \) is the normal probability density function, and \( \Phi(\cdot) \) is the normal cumulative distribution function. By maximizing the \( \text{E}[I(x)] \), we may search a global optimum point with a large probability.

Generally speaking, the least initial sample (design size is \( N = 2(d + 1) \)) is generated by
Latin Hypercube Design for d-dimensionality function. And then, searching an optimal point is done throughout maximizing expected improvement. If maximum evaluation time is met or the maximum EI is less than Tol*minf, stop, or else, reconstruct Kriging and repeat the above step.

However, it is sometimes difficult for EGO to avoid trapping into local optimal area for some optimization problem. In addition, modeling time spent will rapid increase with the introduction of more sampling data or iterations. So a new ISC (i.e., generalized expected improvement) of EGO method is proposed to solve these problems in the following.

ii. Generalized EGO (GEGO) method

As is well known, the standard error \( s \) calculated by DACE (Design and Analysis of Computer Experiments) is slightly lower than its real value. And lower estimated value will result in paying more attention to the exploitation of a local scope until this uncertainty at the region becomes very low, which may lead to ignoring a more global optimization search. Therefore, Generalized Expected Improvement (GEI) [14] was introduced to perform more global explorations. Let \( f_{\text{min}} \) be minimum feasible value of current function \( y = f(x) \), the response is treated as a realization of a random variable \( Y(x) \). The improvement using integer parameter \( g \) over the current best point is defined as

\[
I^g = \max \{0, (f_{\text{min}} - \hat{Y})^g\} \tag{8}
\]

Using Kriging model to predict \( \hat{y} \) and \( \hat{s} \) at the current optimal point, the GEI can be expressed by

\[
E(I^g) = s^g \sum_{k=0}^{g} (-1)^k \frac{g!}{k!(g-k)!} \left( \frac{f_{\text{min}} - \hat{y}}{\hat{s}} \right)^{g-k} T_k \tag{9}
\]

The initial conditions for Eq. (9) are \( T_0 = \Phi(\frac{f_{\text{min}} - \hat{y}}{\hat{s}}) \) and \( T_1 = -\Phi(\frac{f_{\text{min}} - \hat{y}}{\hat{s}}) \), and for \( k > 1 \), \( T_k \) can be recursively calculated by

\[
T_k = -\left( \frac{f_{\text{min}} - \hat{y}}{\hat{s}} \right)^{k-1} \phi \left( \frac{f_{\text{min}} - \hat{y}}{\hat{s}} \right) + (k-1)T_{k-2} \tag{10}
\]

Although Eq. (10) seems to be complicated, its recurrence relationship is simpler to perform. Generally speaking, \( s \) is zero at sampled points and is larger in regions faraway from all sampled points, so the increase of \( g \) tends to result in a more global exploration. In addition, global search often makes large EI have small probability, and local search usually makes small EI have large probability. With the increase of value \( g \), larger EI will be generated and more
global search will be implemented even if they have small probability. Accordingly, a low $g$ value may be apt to sink deeper into a local search. Hence, parameter $g$ value can control the search direction of EGO method in a large part. However, too high $g$ value will not obtain a better solution within a limited number of iterations. On the contrary, too low $g$ value will trap in a local region, which may ignore some high-uncertainty area. For these problem, M. J. Sasena et al. [15] and W. Ponweiser et al. [16] use cooling schedule (Table 1) as cool criterion to choose different $g$ values for different iterations. Similarly to EGO, the flowchart of GEGO can be simply expressed as Fig. 1.

Table 1 Cooling Schedule

<table>
<thead>
<tr>
<th>Iteration</th>
<th>$g$ value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-4</td>
<td>20</td>
</tr>
<tr>
<td>5-9</td>
<td>10</td>
</tr>
<tr>
<td>10-19</td>
<td>5</td>
</tr>
<tr>
<td>20-24</td>
<td>2</td>
</tr>
<tr>
<td>25-34</td>
<td>1</td>
</tr>
<tr>
<td>≥35</td>
<td>0</td>
</tr>
</tbody>
</table>

VI. IMPROVED GENERALIZED EGO METHOD

Seen from cooling schedule (Table 1) in GEGO, it only uses some constant values to replace parameter $g$ for different iterations, which is not able to better describe the behavior and character of generalized expected improvement. So it is necessary for us to find a more appropriate parameter to replace $g$ value. As a key parameter of Kriging model, use of optimal $\theta$ may be wise choice in global optimization process. Therefore, an improved method is present and explained in next sections.

i. IEGEO flow

We present a new method named Improved Generalized Efficient Global Optimization (IEGEO), which mainly integrates the GEI, Kriging model and parameter $\theta$. The flowchart of IEGEO method is shown in Fig. 2. Specific steps are described as follows.
Step 1: Initial experiment design. In order to ensure the stability and uniformity of the spatial distribution, LHD (a space-filling experiment design) is adopted to at least obtain $2(n+1)$ initial sampling points in $n$-dimensional optimization problem, and then, the corresponding responses are evaluated by some function or real-time simulation. It is noted that too much initial sampling data may reduce initial $\theta$ value of Kriging model, which is not suitable for performing a more global searching.

Step 2: Kriging modeling. In addition to the initial DACE modeling, Kriging model will be created by the DACE method.

Step 3: As a key parameter of Kriging model, optimal value $\theta$ will be fetched from the latest Kriging model by Eq. (4). And then, we use the difference between last optimal value $\theta$ and the latest optimal $\theta$ and round off its Euclidean norm as $g$ value in infill sampling criterion. Specific description will be discussed in Section 4.2.

Step 4: Construct GEI. According to Eqs. 8 - 10, we should construct GEI as new infill
sampling criterion so as to find a more promising design point.

**Step 5:** Find next optimal point. Using the constructed Krigeing model, the optimal point with the maximum GEI (Eq. 7) is selected as next optimal sampling point. The choice of $g$ value in GEI will be discussed in detail in Section 4.2.

**Step 6:** Termination criterion. The loop process with modeling, evaluation and optimization will be terminated once the corresponding termination is met. Generally speaking, if generalized expected improvement is less than 0.1% of the current best objective function value or total number of expensive evaluation reaches a fixed value, we will stop the loop. Or else, we will add the new design point with maximum GEI to sample and go on performing next iterate. In this paper, we choose fixed value as termination criterion in order to easily do visualization comparison.

**Step 7:** If Step 6 is not met, the new sampling point will be joined in sample, then go back Step 2.

Then, some key points of the IGEGO method will be discussed in details.

ii. Selection of $g$ value

The reason that we need round off Euclidean norm of variation on the optimal solutions of parameter $\theta$ as $g$ value may be explained by the following issues. First, parameter $\theta$ is a key factor, Krigeing model and other corresponding parameter can be obtained by the parameter with the help of data sample. In addition, when parameter $\theta$ is a larger value, relatively active Krigeing model will make model curve perform a big fluctuations (‘activity’ of the variable $x$ is big), which is helpful for Krigeing model to search more global area. On the contrary, a smaller value for parameter $\theta$ can reduce activity of Krigeing model, which may make exploration sink deep into a local area. Therefore, the change of parameter $\theta$ directly guides whether the optimal searching direction into a more promising area or not. That is why parameter $\theta$ may better control the search space in contrast with parameter $g$ in GEGO. What’s more, correlation function $R(\theta, x_i, x_j)$ in Eq. 2 is usually Gaussian correlation function, i.e., $R(\theta, x_i, x_j) = \exp[-\theta(x_j - x_i)^2]$. In this case, when the distance between two design points in a search is smaller, larger $\theta$ value may result in a very small correlation, which is helpful for current model to jump out of the present local region. Similarly, when the distance is larger, smaller $\theta$ value may also generate high correlation, which may be possible for us to find next
optimal function value in current local area. To sum up, these are why we round off Euclidean norm of $\theta$ as $g$ value to replace $g$ value in Table 1. So improved $g$ value can be expressed as $g = \text{round}(\text{norm}(\theta_{r+1}^* - \theta_i^*))$, \hfill (11)

where $\theta_{r+1}^*$ and $\theta_i^*$ is respectively the optimal values (maximum likelihood estimates) of last parameter $\theta$ and the current parameter $\theta$. The $\text{norm}()$ is Euclidean norm of $(\theta_{r+1}^* - \theta_i^*)$, effect of $\text{round}()$ is deleting the fractional part of $\text{norm}()$, integer parameter $g$ is introduced by GEI (Section 3.2).

Fig. 3 Functional relationship between the number of sampling points and parameter $\theta$ ($\theta = [\theta (1), \theta (2)]$) for the Goldstein Price function

Fig. 3 and Fig. 4 shows functional relationship between the number of sampling points and optimal parameter $\theta$ for the Goldstein Price and Himmelblau function($\theta = [\theta (1), \theta (2)]$). New sampling points are obtained by maximizing ISC. It is obvious that the fluctuation of $\theta (1)$ and $\theta (2)$ is drastic in initial period, which may be suitable for us to search more global region in initial period of evaluations. And their change in fluctuation is also similar. It is noted that changing trends of each element in $\theta$ is almost the same as that of its norm after a great deal of experiments.
With the increase of sampling data, optimal parameter $\theta$ gradually becomes more and more stable, and appears many constant values in big sampling intervals. It means that optimization process gradually tend to local optimal region. However, optimal parameter $\theta$ has some change now and then in the stable process, which may be helpful to search more global region. So it is beneficial for Eq. (11) to act as parameter $g$. To sum up, what we need is the parameter $\theta$ that effectively balances global and local search behavior, so the Eq. (9) is feasible and can be used in IGEGO method.

V. TEST

In section 4, The IGEGO method has been discussed. But its effectiveness and applicability need be further checked and tested for different dimensions of problems. First, six two-dimensional test functions, six multidimensional test functions and an engineering problem (a cycloid gear pump problem) are respectively selected to show superiority of IGEGO method in contrast with GEGO, K-GA (a optimization method based Kriging model and Genetic algorithm [19]) and HAM (Hybrid and adaptive meta-model-based global optimization) [20] for global optimization. Meanwhile, time spent of IKM in IGEGO is compared with that of GEGO. All tests are performed in Matlab 2011a by a Dell machine with i3-2120 3.3GHz CPU and 2GB RAM.

i. Two-dimensional problems

Six two-dimensional test functions including low or high nonlinear and single or multimodal problem are chosen as follows. Their global points and optimal values are shown in Table 2.
(1) Branin function

\[ f(x_1, x_2) = a(x_2 - bx_1^2 + cx_1 - r)^2 + s(1-r)\cos(x_1) + s, \quad x_1 \in [-5, 0], \ x_2 \in [10, 15] \]

The recommended values: \( a = 1, \ b = 5.1/(4\pi^2), \ c = 5/\pi, \ r = 6, \ s = 10 \) and \( t = 1/(8\pi) \).

(2) Goldstein and Price (GP) Function

\[ f(x_1, x_2) = (1 + (x_1 + x_2 + 1)^2(19 - 14x_1 + 3x_1^2 - 14x_2 + 6x_1x_2 + 3x_2^2)) \times ((30 + (2x_1 - 3x_2)^2(18 - 32x_1 + 12x_1^2 + 48x_2 - 36x_1x_2 + 27x_2^2)), \]

\[ x_{1,2} \in [-2, 2] \]

(3) Schaffer Function

\[ f(x_1, x_2) = 0.5 + \frac{\sin^2\left(\sqrt{x_1^2 + x_2^2}\right) - 0.5}{1 + 0.001(x_1^2 + x_2^2)^2}, \quad x_{1,2} \in [-2, 2] \]

(4) Six-hump Camel Back (SCB) Function

\[ f(x_1, x_2) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4, \quad x_{1,2} \in [-2, 2] \]

(5) Himmelblau function

\[ f(x_1, x_2) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2, \]

\[ x_{1,2} \in [-6, 6] \]

(6) Shubert function

\[ f(x_1, x_2) = \left( \sum_{i=1}^{5} \left( i \cos((i+1)x_1 + i) \right)^* \times \left( \sum_{i=1}^{5} \left( i \cos((i+1)x_2 + i) \right) \right) \right), \quad x_{1,2} \in [-10, 10] \]

Table 2 Global points and optimum known for six two-dimensional test functions

<table>
<thead>
<tr>
<th>Test function</th>
<th>Global point(s)</th>
<th>Global optimum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Branin</td>
<td>(-\pi, 12.275)</td>
<td>0.397887</td>
</tr>
<tr>
<td>GP</td>
<td>(0, -1)</td>
<td>3</td>
</tr>
<tr>
<td>Schaffer</td>
<td>(0, 0)</td>
<td>0</td>
</tr>
<tr>
<td>SCB</td>
<td>2 global points</td>
<td>-1.0316</td>
</tr>
<tr>
<td>Himmelblau</td>
<td>4 global points</td>
<td>0</td>
</tr>
<tr>
<td>Shubert</td>
<td>18 global points</td>
<td>-186.7309</td>
</tr>
</tbody>
</table>
To illustrate the 2-D test problems, twelve initial sampling points respectively obtained by LHD will be used to build initial Kriging model. The whole optimal process will be terminated when the total number of expensive evaluation reaches 50.

For 50 expensive evaluations in IGEGO, it is not all global optimization results are good enough. So the better optimization results are shown in Fig. 5 - Fig. 10 for the contours and all expensive evaluation points of the six test functions. In these figures, initial sampling points are signed by '*', other sampling points obtained by ISC are marked with □, and ◊ stands for global optimal point of objective function.

Fig.5 Contours and expensive evaluation points of Branin function

Fig.6 Contours and expensive evaluation points of GP function
Fig. 7 Contours and expensive evaluation points of Schaffer function

Fig. 8 Contours and expensive evaluation points of SCB function

Fig. 9 Contours and expensive evaluation points of Himmelblau function

Seeing from the previous five figures, IGEGO method in most case can escape from some local region and find a minimal point being quite close global optimal value in a more global exploration area. Although bigger region searching is not done in the last figure and some test results is not satisfying, the Shubert function having 18 global minimum can also find a satisfying value in some case.

Next, in order to analyze the efficiency, robustness and applicability of the present method,
three optimization methods (GEGO, K-GA and HAM) based on surrogate model are also employed on the test problems. GEGO method has been introduced in Section 3.2. K-GA is a metamodel optimization method using Kriging model and GA. It can be stated as follows: (1) use initial experiment design to fit a Kriging model, (2) employ GA to find a minimal point of Kriging model, (3) add the optimal point to sample, (4) update Kriging model and loop till total evaluation number is met. The HAM algorithm is also efficient optimization method based on hybrid metamodels (Kriging, RBF and PRS).

![Contours and data points of Shubert function](image1.png)

**Fig.10** Contours and expensive evaluation points of Shubert function

For each test problem, we will perform 10 trials so that the effects of random error will be reasonably lessened. For each numerical trials of 2-D function, the four optimization methods will be terminated once the number of expensive evaluation arrives at 50, which also includes the number of objective function evaluation in initial sampling. In addition, all two-dimensional problems will use the same initial sampling points so as to reduce the influence of initial experiment design for different optimization algorithms.

![Optimization results of Branin function](image2.png)

**Fig.11** Optimization results of Branin function

Optimization results of the six 2-D test functions for different optimization methods are shown in Fig. 11 - Fig. 16. In these figures, the abscissa is the number of numerical tests (10 trials), and the ordinate is \( y^* - y_{best} \), where \( y^* \) is the approximate global minimum obtained by
optimization algorithm, and $y_{\text{best}}$ is global optimal value of objective function.

Fig. 12 Optimization results of GP function

Fig. 13 Optimization results of Schaffer function

Fig. 14 Optimization results of SCB function

Diagnostic test results throughout 50 function evaluations show that the IGEGO method perform better than GEGO, K-GA and HAM on GP, Schaffer and Shubert function, and slightly better than GEGO and K-GA on Branin, SCB and Himmelblau functions. For the six test functions, IGEGO can always find a better minimum in one time or several times of 10 trials, and the optimal value found by IGEGO is usually superior to other three optimization methods,
which is what we expected. By contrast, the results of HAM algorithm is not very well in the same conditions for 2-D problems, but it may be more suitable for high-dimensional problem according to the next test results. Moreover, Optimization results (Fig.12 and Fig. 16) on GP and Shubert function have bigger absolute error in most trials. Two reasons may explain the problem. On the one hand, corresponding logarithmic deformation should be done to improve optimization results because expression of the two functions is the product of relationship. On the other hand, the two functions is high-nonlinear (include many extreme points), accordingly, introduction of the added expensive evaluation points is necessary in order to enhance stability probability of test results in global optimization process. In a word, 50 expensive evaluations can make the proposed method obtain global optimal values for most 2-D problem.

![Graph](image1.png)

**Fig.15 Optimization results of Himmelblau function**

![Graph](image2.png)

**Fig.16 Optimization results of Shubert function**

### ii. Multi-dimensional problems

Six multi-dimensional test functions are chosen as follows. Their dimension, global points and optimal values are shown in Table 3, and $N_{\text{max}}$ is maximum evaluation number.

1. Hartman3 function
\[ f(x) = -\sum_{i=1}^{4} \alpha_i \exp \left( -\sum_{j=1}^{3} A_{ij} (x_j - P_{ij})^2 \right), \]
\[ x_i \in [0,1], \ i = 1,...,3 \]

where, \( \alpha = (1.0, 1.2, 3.0, 3.2)^T \)
\[ A = \begin{bmatrix} 3.0 & 10 & 30 \\ 0.1 & 10 & 35 \\ 3.0 & 10 & 30 \\ 0.1 & 10 & 36 \end{bmatrix}, \]
\[ P = 10^{-4} \begin{bmatrix} 3689 & 1170 & 2673 \\ 4699 & 4387 & 7470 \\ 1091 & 8732 & 5547 \\ 381 & 5743 & 8828 \end{bmatrix} \]

(2) Shekel10 function

\[ f(x) = -\sum_{i=1}^{10} \left( -\sum_{j=1}^{4} (x_j - C_{ij})^2 + \beta_j \right)^{-1}, \]
\[ x_i \in [0,10], \ i = 1,...,4 \]

where, \( \beta = (0.1, 0.2, 0.2, 0.4, 0.4, 0.6, 0.3, 0.7, 0.5, 0.5)^T \),
\[ C = \begin{bmatrix} 4 & 1 & 8 & 6 & 3 & 2 & 5 & 8 & 6 & 7 \\ 4 & 1 & 8 & 6 & 7 & 9 & 3 & 1 & 2 & 3 \\ 4 & 1 & 8 & 6 & 7 & 9 & 3 & 1 & 2 & 3 \end{bmatrix} \]

(3) Hartmann6 function

\[ f(x) = -\sum_{i=1}^{4} \alpha_i \exp \left( -\sum_{j=1}^{6} A_{ij} (x_j - P_{ij})^2 \right), \]
\[ x_i \in [0,1], \ i = 1,...,6 \]

where, \( \alpha = (1.0, 1.2, 3.0, 3.2)^T \)
\[ A = \begin{bmatrix} 10 & 3 & 17 & 3.5 & 1.7 & 8 \\ 0.05 & 10 & 17 & 0.1 & 8 & 14 \\ 3 & 3.5 & 1.7 & 10 & 17 & 8 \\ 17 & 8 & 0.05 & 10 & 0.1 & 14 \end{bmatrix}, \]
\[ P = 10^{-4} \begin{bmatrix} 1312 & 1696 & 5569 & 124 & 8283 & 5886 \\ 2329 & 4135 & 8307 & 3736 & 1004 & 9991 \\ 2348 & 1451 & 3522 & 2883 & 3047 & 6650 \\ 4047 & 8828 & 8732 & 5743 & 1091 & 381 \end{bmatrix} \]

(4) Dixon-Price9 function

\[ f(x) = (x_1 - 1)^2 + \sum_{i=2}^{9} i (2x_i^2 - x_{i-1}), \]
\[ x_i \in [-10,10], \ i = 1,...,9 \]
(5) Rosenbrock10 function

\[ f(x) = -\sum_{i=1}^{9} [100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2], \]
\[ x_i \in [-2, 2], \quad i = 1, \ldots, 10 \]

(6) Rastrigin12 function

\[ f(x) = 120 + \sum_{i=1}^{12} [(x_i^2 - 10\cos(2\pi x_i))], \]
\[ x_i \in [-1, 3], \quad i = 1, \ldots, 12 \]

Table 3 Global optimal data and initial configuration for six multi-dimensional test functions

<table>
<thead>
<tr>
<th>Test function</th>
<th>Hartman3</th>
<th>Shekel10</th>
<th>Hartmann6</th>
<th>Dixon-Price</th>
<th>Rosenbrock10</th>
<th>Rastrigin12</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimenson</td>
<td>3</td>
<td>4</td>
<td>6</td>
<td>9</td>
<td>10</td>
<td>12</td>
</tr>
<tr>
<td>Global point(s)</td>
<td>(0.114614, 4, 4, 3.0169, 0.150011, 0.275332, 0.311652, 0.6573)</td>
<td>(0.20169, 4, 4, 0.275332, 0.311652, 0.6573)</td>
<td>(1, ..., 1)</td>
<td>(0, ..., 0)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Global optimum</td>
<td>-3.86278</td>
<td>-10.53</td>
<td>-3.32237</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Initial sample</td>
<td>14</td>
<td>18</td>
<td>25</td>
<td>36</td>
<td>41</td>
<td>50</td>
</tr>
<tr>
<td>N_max</td>
<td>60</td>
<td>70</td>
<td>80</td>
<td>120</td>
<td>150</td>
<td>180</td>
</tr>
</tbody>
</table>

Optimization results on the six multi-dimensional functions for different optimization methods are shown in Fig. 17 - Fig. 22.

For Hartman3 and Shekel10 functions, results obtained by the four algorithms are satisfactory in general. In Hartman3, IGEGO and GEGO have similar results, and K-GA and HAM have a little bad. But they can basically find approximate optimal values \( y^* \) close to real optimums \( y_{best} \).

In Shekel10, the absolute error \( (y^* - y_{best}) \) of \( y^* \) acquired by GEGO, K-GA and HAM are all
greater than 1 in 10 trials. But IGEGO can search better $y^*$ (absolute error is less than 1) in two times of 10 trials.

For Hartman6 function, optimization results of the four algorithms are clearly divided into two parts. Therefore, for this type of function, optimizing GEI filling sampling criteria with IGEGO and GEGO to get next best point may be a wise choice.
convergence. For Dixon-Price9 function, we have found global optimum which absolute error is smaller in some trials. In the optimal process, K-GA is not good, IEGEO is slightly better than GEGO and HAM.

For Rosenbrock10 and Rastrigin12 functions, four methods are not doing well. HAM algorithm slightly shows its superiority of handling high dimension problem in some trials. These absolute errors are not what we expect. Especially for Rastrigin12 function, we sequentially increase more evaluation points in several tests and discover that the optimal point is hardly any significant improvement.

![Fig. 20 Optimization results of Dixon-Price9 Function](image1)

![Fig.21 Optimization results of Rosenbrock10 function](image2)
The number of numerical tests $y^*-y_{best}$

**Rastrigin12 function**

IGEGO

GEGO

K-GA

HAM

![Fig. 22 Optimization results of Rastrigin12 function](image)

Thus, we think that IGEGO and GEGO methods are not suitable for the optimization problem which dimension is more than 10. After all, it is difficult for Kriging model to perform high-dimensional model approximation in general. To sum up, it is appropriate for IGEGO method to explore a global optimal solution for 1-10 dimensional problems.

**iii. Engineering problems**

In this section, the structural optimization design of cycloid gear pump will be realized by IGEGO method. Cycloid gear pump is composed of the inner rotor and the outer rotor, the front cover, the back cover and the shell. The sketch of cycloid gear pump is shown in Fig. 23. $W_1$ and $W_1'$ are two symmetrical meshing points between two sides of some tooth of the inner rotor and two teeth of the outer rotor when the inner and outer rotors have the minimum area. $W_2$ and $W_2'$ are also two meshing ones between the two teeth of the inner rotor and the two sides of the outer rotor when the area is maximized. The four points are the theoretical reference positions, according to the tooth curves of cycloid gear pump and engagement theory, theoretical value of the closed-line angles can be calculated by reference [21].

![Fig. 23 Sketch on inlet and outlet cavities of cycloid gear pump](image)
In order to increase actual flow, for $\alpha_0$ side (having a big oil cavity), we should turn off oil inlet cavity later so that more oil is entered (i.e., $\alpha_0 > \alpha_1$); considering that throttling, we should turn on the oil outlet cavity in advance ($\alpha_0 > \alpha_2$). Likewise, for $\beta_0$ side (having a small oil cavity), since the sealing zone is very small, the width of the sealing zone should be increased, therefore, we expect opening size ($\beta_1$) of the oil inlet cavity and closing size ($\beta_2$) of the oil outlet cavity are both slightly larger than $\beta_0$. The actual flow will be directly affected by changing of the four meshing angles. The internal flow field of cycloid gear pump is numerically simulated by computational fluid dynamics (CFD) model to obtain a bigger average volume flux in outlet. It is beneficial for cycloid gear pump to enhance its volume efficiency within a certain range.

According to the above analysis, we respectively set the four geometric angles (i.e. $\alpha_1$, $\alpha_2$, $\beta_1$ and $\beta_2$) in inlet and outlet and average volume flux as input variables $x_1, x_2, x_3, x_4$ and output variable $y$ in the case of a fixed rotation speed (3000r/min). Under ideal conditions, the four variables are $x_1, 2=26^\circ$ and $x_3,4=13.2^\circ$, which are obtained from the above closed-line angles formula according to the geometry size of cycloid gear pump. Meanwhile, the theoretical flow $Q_0 = 3.22$ L/min can also be obtained from approximate calculation formula of cycloid gear pump. But values of the four variables should be improved to further enhance volume efficiency in actual real engineering simulation. Therefore, in accordance with the design idea, the engineering optimization problem can be stated as follows:

$$\begin{align*}
\min & \quad -y \\
\text{s.t.} & \quad 22 \leq x_{1,2} \leq 26 \\
& \quad 13.2 \leq x_{3,4} \leq 16.2
\end{align*}$$

(12)

These variables or output has been explained. In the optimization problem, as CFD model of internal flow field in cycloid gear pump, the objective function is black-box. The CFD model can be built by the following steps: (1) use Pro/E to build a geometric model of internal flow.
field (2) the geometric model will be imported into pretreatment module of Pumplinx™ with STL format. Meshing results of internal flow field is shown in Fig. 24 after splitting, merging and grouping calculation domain of the flow field.

We set the simulation time of this CFD model as 0.2 sec, in this case, about fifty minutes should be spent to finish the real simulation. Moreover, we set the maximum simulation number as 40, which will spend on 33 hours in the whole optimization. In addition, the IGEGO and GEGO methods are adopted to deal with the black-box optimization problem. In the light of the above conditions, 10 initial sampling points are chosen to construct the simulation model, and optimization process will be terminated until total evaluation number reaches 40. Initial optimal value of average volume flux is 2.3670 L/min, corresponding volume efficiency is 73.51%. Results on optimization process of the two methods are shown in Fig. 25. The best average volume flux and corresponding volume efficiency are listed in Table 4. It is obvious that the IGEGO method can find a bigger average volume flux, and volume efficiency obtained by IGEGO has increased about 2.07% against that of GEGO.

![Graph showing optimization results](image)

Fig. 25 Optimization results on average volume flux in outlet for different simulation evaluation number

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Initial Design</th>
<th>IGEGO</th>
<th>GEGO</th>
</tr>
</thead>
<tbody>
<tr>
<td>((x_1, x_2, x_3, x_4))</td>
<td>(26, 26, 13.2, 13.2)</td>
<td>(24.34, 24.76, 15.40, 15.85)</td>
<td>(25.70, 24.78, 14.30, 13.83)</td>
</tr>
</tbody>
</table>
VI. Conclusions

A new EGO method named IGEGO is present from optimization effect. In this method, a new infill sampling criterion called GEI which round off Euclidean norm of difference of the maximum likelihood estimate of parameter $\theta$ to replace parameter $g$ can effectively balance global and local search. Moreover, Kriging model can adaptively offer a suitable approximation model so as to help IGEGO perform a good optimization. The two key points ensure the applicability, effectiveness and reliability of the proposed methods, which has been investigated and verified by twelve numerical test problems and an engineering simulation example. From the results, we can draw the following conclusions.

1) IGEGO method is able to explore a better global optimal solution under the same conditions of evaluation, in other words, the probability of finding the global optimum is higher than the other three optimization algorithms due to the randomness of the optimization process.

2) For test problems which dimensions are less than 10, IGEGO method could effectively finish global optimization tasks. Apart from this, using the proposed method may not be a good choice because Kriging model may be not suitable for the establishment of high-dimensional models.

As an additional discussion, how to handle constraint optimization problem based on surrogate model may be researched by considering disposal of constraint problem, the choice of feasible sampling point, how to use appropriate ISC and termination rule etc.
ACKNOWLEDGEMENT

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