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## Sequential RBF Surrogate-based Efficient Optimization Method for Engineering Design Problems with Expensive Black-Box Functions

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**Abstract:** As a promising technique, surrogate-based design and optimization (SBDO) has been widely used in modern engineering design optimizations. Currently, static surrogate-based optimization methods have been successfully applied to expensive optimization problems. However, due to the low efficiency and poor flexibility, static surrogate-based optimization methods are difficult to efficiently solve practical engineering cases. At the aim of enhancing efficiency, a novel surrogate-based efficient optimization method is developed by using sequential radial basis function (SEO-SRBF). Moreover, augmented Lagrangian multiplier method is adopted to solve the problems involving expensive constraints. In order to study the performance of SEO-SRBF, several numerical benchmark functions and engineering problems are solved by SEO-SRBF and other well-known surrogate-based optimization methods including EGO, MPS, and IARSM. The optimal solutions, number of function evaluations, and algorithm execution time are recorded for comparison. The comparison results demonstrate that SEO-SRBF shows satisfactory performance in both optimization efficiency and global convergence capability. The CPU time required for running SEO-SRBF is dramatically less than that of other algorithms. In the torque arm optimization case using FEA simulation, SEO-SRBF further reduces 21% of the material volume compared with the solution from static-RBF subject to the stress constraint. This study provides the efficient strategy to solve expensive constrained optimization problems.

**Keywords:** surrogate-based optimization, global optimization, significant sampling space, adaptive surrogate, radial basis function

### 1 Introduction

Essentially, most optimizations for modern engineering designs are challenging tasks since very limited information on simulation models (e.g., continuity, differentiability, convexity, etc.) is known *a priori*. Due to the lack of transparency, such simulation models are often referred to as black-box functions. Furthermore, complex systems consisting of several internally coupled subsystems frequently appear in modern engineering design. For example, in aircraft design process, aerodynamic, structure, propulsion, control, stealth, and some other disciplines need to be considered. Multidisciplinary design optimization (MDO) has been frequently employed to improve the design quality and reduce the probability of redesign. To enhance the accuracy and reliability of the design results, high fidelity analysis and simulation models have been widely applied in today's engineering design. For instance,

the aerodynamic and structure characteristics are usually evaluated by using computational fluid dynamics (CFD) models and finite element analysis (FEA) models, respectively. Although improvement of analysis accuracy can be achieved by using such expensive models, the high fidelity analysis models are computationally expensive, and the elapsed time required for simulation is dramatically increased. It generally takes several or even more than tens of hours to run a CFD aerodynamic simulation. Because of the iterative behavior of optimization process, analysis models have to be invoked more than thousands of times by using traditional global optimization algorithms, such as generic algorithm (GA)<sup>[1]</sup> and simulated annealing (SA)<sup>[2]</sup>. In addition, for each system-level analysis of coupled complex problems, all the analysis models of subsystems need to be repeatedly performed to meet interdisciplinary compatibility. Thus, it is rather time-consuming to perform modern engineering design optimizations by directly using the conventional global optimization algorithms and computationally expensive analysis models. For the purpose of alleviating the computational burden, surrogate-based design and optimization (SBDO)<sup>[3]</sup> has been developed.

Through replacing computation-intensive models with surrogates, we can significantly reduce the computation cost for reaching the true global optimum. So far, various surrogate approaches have been developed, such as

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Response Surface Method (RSM), Radial Basis Function (RBF)<sup>[4-5]</sup>, Kriging(KRG)<sup>[6]</sup>, and so on. Those surrogate technologies have been reviewed by WANG and SHAN<sup>[3]</sup>, and YOUNIS and DONG<sup>[7]</sup>. JIN, et al<sup>[8]</sup>, systematically compared the performance of RSM, RBF, KRG and Multivariate Adaptive Regression Splines(MARS) under different criteria including prediction accuracy, computational cost and robustness, and pointed out that RBF shows the good overall performance. RBF surrogate performs pretty efficiently in practice due to the easily adjustable smoothness and powerful convergence properties<sup>[7]</sup>. GUTMANN<sup>[9]</sup> summarized most kinds of RBF and proposed an adaptive RBF method for global optimization using P-algorithm. Furthermore, recently RBF surrogate have been applied in practical engineering designs and optimizations<sup>[10-11]</sup>.

Because it is difficult to build an accurate static surrogate with small scale samples in large design space, especially for high dimensional functions with high nonlinear behavior, static surrogate-based optimization methods requires a large amount of samples to guarantee the global approximation accuracy and avoid missing the true global optimum<sup>[12-13]</sup>. To further improve the optimization efficiency, adaptive or dynamic surrogate-based optimization methods have drawn more and more attention. In recent years, many studies on adaptive surrogate-based optimization have been reported. A brief summary is presented as follows. JONES, et al<sup>[14]</sup>, proposed an efficient global optimization(EGO) method that starts with a small scale of samples and positions the additional samples through maximizing the value of expected improvement. During the process, KRG surrogate is reconstructed by using the increasing samples until the expected improvement becomes small enough. Several infill sampling criteria were discussed for EGO<sup>[15]</sup>. ALEXANDROV, et al<sup>[16]</sup>, developed a surrogate management framework using trust region method to update surrogates according to predicted improvement of objective function during the optimization process. In variable fidelity optimization, GANO, et al<sup>[17]</sup>, proposed a surrogate updating management scheme using trust region ratio(TR-MUMS) that compares the approximation to the true model to refine KRG scaling model. HAFTKA<sup>[18]</sup> introduced variable complexity modeling(VCM) method and applied it to optimize a high-speed civil transport. Adaptive response surface method(ARSM) using cutting plane approach for design space reduction has first proposed by WANG, et al<sup>[19]</sup>. An improved ARSM<sup>[20]</sup> using inherited LHD sampling method is then developed to reduce the number of expensive function evaluations. Based on ARSM, WONG and WANG<sup>[21]</sup> presented a DFP methodology to minimize production costs of industry products. PANAYI, et al<sup>[22]</sup>, developed pseudo-ASRM using iteratively weighted least-squares to enhance the approximation accuracy, which was applied to optimize piston skirt profiles. WANG and SIMPSON<sup>[23]</sup> developed

fuzzy c-mean clustering to reduce the design space, and in the reduced design space sequential samples were increased to update KRG surrogate until convergence. WANG, et al<sup>[24]</sup>, proposed mode pursuing sampling(MPS) method to discriminatively produce more samples towards the global optimum. Furthermore, a discrete variable MPS(D-MPS)<sup>[25]</sup> using a double-sphere strategy to balance exploration and exploitation samples was developed for discrete variable optimization problems. SI-MO developed by MULLER, et al<sup>[26]</sup>, iteratively evaluates the computationally expensive simulation at four chosen points from the groups to update RBF surrogate. To improve the accuracy of RBF, KITAYANMA, et al<sup>[27]</sup>, studied the width factor of basis functions and proposed a sequential approximate optimization(SAO) procedure. CONN and LE<sup>[28]</sup> applied quadratic models with mesh adaptive direct search for constrained black box optimization.

Domestic researchers have also conducted some studies in SBDO field. LONG, et al<sup>[29]</sup> proposed an enhance adaptive response surface method(EARSM) using significant design space(SDS) method to identify the design space of interest, which probably contains the global optimum. And then EARSM is applied to solve aero-structure coupled optimization of a high aspect ratio wing<sup>[30]</sup>. ZHU, et al<sup>[31]</sup>, developed a new global optimization method using successive local enumeration (SLE) and adaptive RBF based on fuzzy clustering. LI, et al<sup>[32]</sup>, proposed a novel surrogate-based global optimization strategy using fuzzy clustering for design space reduction. Based on SBDO technology, PENG, et al<sup>[33]</sup>, developed an efficient truss structure optimization framework using CAD/CAE integration. YOUNIS and DONG<sup>[7]</sup> reviewed a number of popular global optimization methods for black-box functions. More detailed information about SBDO can be found in the valuable surveys<sup>[3, 7, 34-35]</sup>.

A novel surrogate-based efficient optimization strategy with sequential radial basis function(SEO-SRBF) is proposed for the purpose of improving the efficiency and capability of searching global optimum for engineering optimization problems involving both expensive objective function and constraints.

The rest of this article is organized as follows. In section 2, the algorithm and procedure of SEO-SRBF are presented in detail, especially for the significant sampling space(SSS) method. In section 3, the proposed SEO-SRBF is applied to solve several numerical benchmark problems and two practical engineering optimization problems, and comparative studies with other SBDO methods are also conducted to demonstrate the merits of SEO-SRBF. In section 4, further discussion on SEO-SRBF is presented. In the last section, concluding remarks.

## 2 Sequential Radial Basis Function

### 2.1 Design and analysis computer experiment

Design and Analysis of Computer Experiment(DACE) is

a key technique for SBDO methods. For the purpose of improving approximation accuracy of surrogates, the DACE methods are desired to generate samples with good performances in both space-filling and the projective properties<sup>[36]</sup>. To meet the space-filling requirement, Maximin Distance design<sup>[37]</sup> has been developed to maximize the minimum distance among all samples. To achieve projective property, the Latin Hypercube Design (LHD) is proposed by MCKAY, et al<sup>[38]</sup>. And to make the samples evenly spread in the design space, several optimal LHD methods under various criteria including maximin distance,  $CL_2$  and  $\phi_p$  have been studied, such as optimal LHD method using simulated annealing algorithm<sup>[39]</sup>, threshold accepting algorithm<sup>[40]</sup>, enhanced stochastic evolutionary algorithm<sup>[41]</sup> and SLE<sup>[31]</sup>.

SEO-SRBF employs *lhsdesign* function provided in MATLAB with maximin criterion to produce samples for the three reasons below: 1) More information within a design space would be offered by LHD; 2) The size of LHD samples is controllable<sup>[20]</sup>; 3) For adaptive SBDO methods, generation of sequential samples closer to the global optimum is more effective than producing evenly distributed initial samples by using the complicated optimal LHD methods.

## 2.2 Radial basis function

Radial basis function(RBF) is one of the multi-dimensional interpolation methods based on scattered data, which has been widely used as the surrogate for approximating the computation-intensive functions. The basic formulation of RBF is expressed as follows:

$$\begin{cases} f_r(x) = \sum_{i=1}^{n_s} (\beta_r)_i \phi(\|x - x_i\|) = \beta_r^T \boldsymbol{\phi}, \\ \boldsymbol{\phi} = \left( \phi(\|x - x_1\|), \dots, \phi(\|x - x_{n_s}\|) \right)^T, \\ \beta_r = \left( (\beta_r)_1, \dots, (\beta_r)_{n_s} \right)^T, \end{cases} \quad (1)$$

where radial function  $\boldsymbol{\phi}$  is a set of functions based on Euclidean distance  $\|x - x_i\|$ .  $\beta_r$  is the vector of linear weight coefficients.  $n_s$  is the number of samples.  $\beta_r$  should satisfy the interpolation conditions as below:

$$(f_r)_i = y_i, \quad i = 1, 2, \dots, n_s, \quad (2)$$

where  $y_i$  and  $(f_r)_i$  are the responses of the true function and RBF surrogate at the sample  $x_i$ , respectively. Therefore,  $\beta_r$  can be determined as follows:

$$A_r \beta_r = y, \quad (3)$$

$$\beta_r = A_r^{-1} y, \quad (4)$$

where  $A_r$  is a matrix given by Eq. (5):

$$A_r = \begin{pmatrix} \phi(\|x_1 - x_1\|) & \dots & \phi(\|x_1 - x_{n_s}\|) \\ \vdots & & \vdots \\ \phi(\|x_{n_s} - x_1\|) & \dots & \phi(\|x_{n_s} - x_{n_s}\|) \end{pmatrix}, \quad (5)$$

$\phi$  is the radial function, and Table 1 summaries the typical radial functions.

**Table 1. Typical RBF functions**

Classical RBF	Equation
Linear	$\phi(r) = cr$
Cubic	$\phi(r) = (r + c)^3$
Thin plate spline	$\phi(r) = r^2 \ln(cr^2)$
Gaussian	$\phi(r) = \exp(-cr^2)$
Multiquadratic	$\phi(r) = (r^2 + c^2)^{1/2}$

The radial distance  $r$  in Table 1 is the Euclidean distance  $\|x - x_i\|$ , and the best value of constant  $c$  in Table 1 is problem-dependent. In SEO-SRBF,  $c$  is set in terms of the empirical formula in Eq. (6):

$$c = \left( \frac{\max(\mathbf{X}) - \min(\mathbf{X})}{n_s} \right)^{\frac{1}{n_v}}, \quad (6)$$

where  $\mathbf{X}$  is the matrix of all the samples, and  $n_v$  is the dimension of design space.

## 2.3 Procedure of SEO-SRBF

SEO-SRBF is proposed for adaptive surrogate-based optimization on engineering optimizations involving expensive models. In general, an engineering optimization problem can be considered as a typical nonlinear optimization problem with a general formulation as shown in Eq. (7):

$$\begin{aligned} \min & f(\mathbf{x}), \\ \text{s.t.} & g_i(\mathbf{x}) \geq 0 \quad (i = 1, 2, \dots, l), \\ & h_j(\mathbf{x}) = 0 \quad (j = 1, 2, \dots, m). \end{aligned} \quad (7)$$

The fitting quality of RBF in the entire design space can be gradually improved as the number of samples increases. Besides, RBF provides more accurate approximation at the neighborhood of the existing samples. In terms of the preceding features of RBF, the novel SEO-SRBF is developed to sequentially add new samples in the significant sampling space(SSS) during the optimization process. By use of the gradually increasing samples, the fitting quality of RBF in significant regions is improved, furthermore, the global optimum of engineering optimization problem could be obtained through running RBF surrogate based optimizations.

The flowchart of SEO-SRBF is shown in Fig. 1. First, designers have to set the initial conditions including design

variables, objective function, design space, number of initial samples  $N_{\text{initial}}$  and number of newly-added samples  $N_{\text{add}}$  at each iteration. The choice of  $N_{\text{initial}}$  and  $N_{\text{add}}$  depends on the complexity of the optimization problem, such as the dimension of design space and nonlinearity. The approach of setting will be discussed in the following sections. Once the initial conditions are configured, global optimization using SEO-SRBF is executed in terms of the following steps.

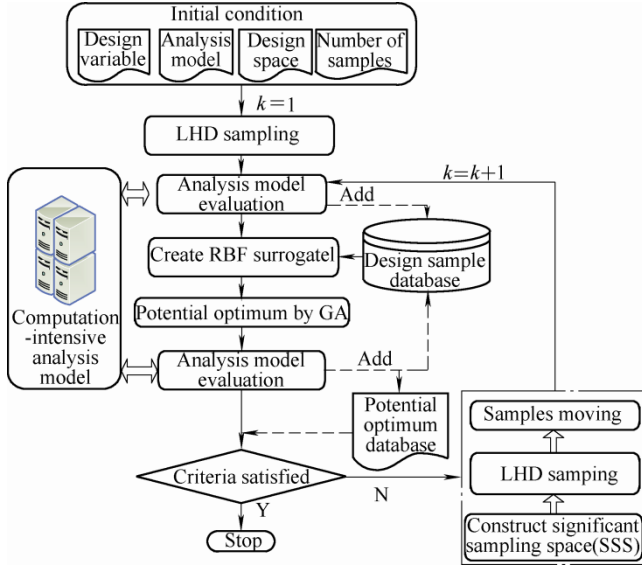


Fig. 1. Flowchart of SEO-SRBF

Step 1. The initial samples  $N_{\text{initial}}$  are generated in the entire design space through LHD sampling with maximin criterion.

Step 2. The responses of true objective function at those initial samples are evaluated by calling the expensive analysis models, and then the initial samples and corresponding objective responses are stored in the design sample database for constructing RBF surrogate in following steps.

Step 3. The RBF surrogate is constructed based on all the samples in current design sample database. During the optimization process, when the size of samples increases, the approximation accuracy of RBF surrogate is enhanced successively.

Step 4. Based on current RBF surrogate, global optimization is performed by using GA to obtain the potential optimum, which is regarded as the best solution under current acquired information about the optimization problem. The response of true objective at the potential optimum is then calculated by evaluating the expensive analysis models, which is stored in the potential optimum database and design sample database, respectively.

Step 5. The termination criterion is used to determine whether the optimization process should be continued. If satisfied, SEO-SRBF optimization is terminated. Otherwise, the process turns to step 6.

Step 6. New samples are generated by using significant sampling space(SSS) method and sequential LHD sampling

method. The new samples and their true objective responses are also stored in design sample database to improve the accuracy of RBF. Optimization process goes back to step 3. The SSS method and sequential LHD sampling method are respectively detailed in the following section.

## 2.4 Significant sampling space method

SSS is a unique technique in SEO-SRBF for enhancing the optimization efficiency and global convergence performance. Significant sampling space is a sub-region around the current potential optimum that probably contains the true global optimum<sup>[42]</sup>. SSS is beneficial to improving the approximation accuracy of RBF in the region near to the true global optimum through sequentially increasing new samples. The procedure of SSS to construct  $k$ th significant sampling space is given in Algorithm 1.

### Algorithm 1: SSS

**Input:**  $k$ th potential optimum  $\mathbf{x}_k^*$ ; objective response at  $k$ th potential optimum  $y_k^*$ ; current design samples set  $\mathbf{X}$ ; objective responses set  $\mathbf{Y}$ ; relative error of objective at the  $(k-1)$ th potential optimum  $\varepsilon_{k-1}$ ; length of  $(k-1)$ th significant sampling space  $\mathbf{B}_{k-1}$ ; coefficient for determining the length of SSS  $\alpha$ ; coefficient for minimum design space  $\sigma$ ; entire design space  $\mathbf{S}_0$ .

**Output:**  $k$ th significant sampling space  $\mathbf{S}_k$ .

```

1 Begin
2   if  $y_k^* < y_{k-1}^*$  or  $k == 1$  then
3      $\mathbf{B}_k \leftarrow \text{EvalLengthSSS}(\mathbf{x}_k^*, \mathbf{x}_{k-1}^*, \mathbf{X})$ 
4      $\varepsilon_k \leftarrow \varepsilon_{k-1}$ 
5      $\mathbf{S}_{\text{center}} \leftarrow \mathbf{x}_k^*$ 
6   else
7      $\varepsilon_k \leftarrow \text{LeaveOneOut}(\mathbf{X}, \mathbf{Y}, \mathbf{x}_k^*, y_k^*)$ 
8     if  $\varepsilon_k < \varepsilon_{k-1}$  then
9        $\mathbf{B}_k \leftarrow \mathbf{B}_{k-1} / \alpha$ 
10    else
11       $\mathbf{B}_k \leftarrow \mathbf{B}_{k-1} * \alpha$ 
12    end
13     $\mathbf{S}_{\text{center}} \leftarrow \mathbf{x}_{k-1}^*$ 
14  end
15   $\mathbf{B}_k \leftarrow \text{CheckMinBound}(\mathbf{B}_k, \sigma, \mathbf{S}_0)$ 
16   $\mathbf{S}_k \leftarrow \text{EvalSSS}(\mathbf{S}_{\text{center}}, \mathbf{B}_k, \mathbf{S}_0)$ 
17 End

```

The current information  $(\mathbf{x}_k^*, y_k^*, \mathbf{X}, \mathbf{Y}, \varepsilon_{k-1}, \mathbf{B}_{k-1}, \alpha, \sigma, \mathbf{S}_0)$  is used as inputs and the  $k$ th significant sampling space  $\mathbf{S}_k$  is returned. Five steps of this algorithm can be summarized as follows.

Step 1(lines 1–5): If the objective response at the current potential optimum is less than that at last iteration (i.e.,  $y_k^* < y_{k-1}^*$ ) or the iterative counter  $k$  equals to 1, the length of  $k$ th SSS is calculated at line 3 by using function  $\text{EvalLengthSSS}()$  in Eq. (8). In that equation, if  $k \geq 2$ , the length is updated in terms of the last two optima, and the  $k$ th relative error  $\varepsilon_k$  is set to the  $(k-1)$ th relative error

$\varepsilon_{k-1}$ . At the first iteration ( $k = 1$ ), the length of SSS is calculated in terms of the first potential optimum and the sample  $\mathbf{x}_{\max}$  with the maximum relative error among all initial samples. The relative error is evaluated by using leave-one-out cross validation scheme<sup>[34]</sup>. The center of  $k$ th SSS is set to the  $k$ th potential optimum  $\mathbf{x}_k^*$  at line 5. The process goes to step 4.

$$\mathbf{B}_k = \begin{cases} \left| \mathbf{x}_k^* - \mathbf{x}_{k-1}^* \right|, & k \geq 2, \\ \left| \mathbf{x}_k^* - \bar{\mathbf{x}}_{\max} \right|, & k = 1. \end{cases} \quad (8)$$

Step 2 (lines 6–7): If the objective response at the current potential optimum is larger than the that at last iteration (i.e.,  $y_k^* \geq y_{k-1}^*$ ), the relative error  $\varepsilon_k$  at the current potential optimum is evaluated by using leave-one-out cross validation.

Step 3 (lines 8–14): If  $\varepsilon_k < \varepsilon_{k-1}$ , the increasing length of  $k$ th SSS is set to  $\mathbf{B}_{k-1}/\alpha$ , otherwise, the length is reduced as  $\mathbf{B}_{k-1} * \alpha$ . And the center of  $k$ th SSS is set to the last potential optimum  $\mathbf{x}_{k-1}^*$ .

Step 4 (line 15): In function *CheckMinBound()*, if the length in any dimension get less than the minimum allowed length (i.e.,  $\mathbf{B}_k < \sigma|\mathbf{S}_0$ ), it is adjusted to the minimum length  $\sigma|\mathbf{S}_0$ . The procedure goes to step 5.

Step 5 (line 16): Through calling function *EvalSSS()*, the  $k$ th trial SSS is expressed by  $\mathbf{S}_k^t = [\mathbf{B}_k^{(L)}, \mathbf{B}_k^{(U)}]$ .  $\mathbf{B}_k^{(L)}$  and  $\mathbf{B}_k^{(U)}$  respectively indicate the lower and upper boundary vectors with  $n_v$  elements, which are identified in Eq. (9). To avoid SSS exceeding the boundary of the initial design space when the current potential optimum locates close to the boundary, the final  $\mathbf{S}_k$  is defined as the intersection part between  $\mathbf{S}_k^t$  and  $\mathbf{S}_0$ , namely  $\mathbf{S}_k = \mathbf{S}_k^t \cap \mathbf{S}_0$ , as illustrated in Fig. 2.

$$\begin{aligned} \mathbf{B}_k^{(L)} &= \mathbf{S}_{\text{center}} - \mathbf{B}_k, \\ \mathbf{B}_k^{(U)} &= \mathbf{S}_{\text{center}} + \mathbf{B}_k. \end{aligned} \quad (9)$$

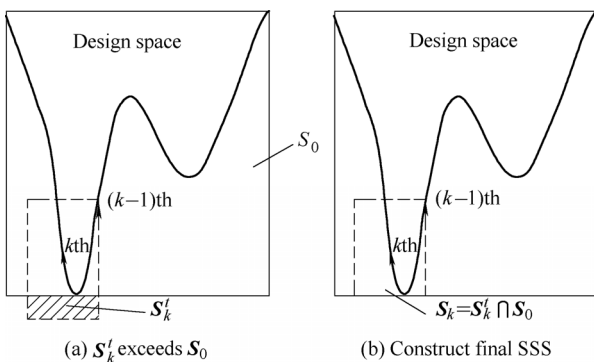


Fig. 2. Illustration of determining SSS

2.5 Termination criterion

In this article, when the relative difference of two consecutive potential optima is less than a predefined

tolerance factor, SEO-SRBF process is terminated and outputs the last potential optimum as the final solution. The termination criterion is shown in Eq. (10), where  $y_k^*$  and  $y_{k-1}^*$  are respectively the values of objective function at  $k$ th and  $(k-1)$ th potential optimum:

$$\left| \frac{f_k^* - f_{k-1}^*}{f_{k-1}^*} \right| \leq \eta. \quad (10)$$

2.6 SEO-SRBF for constrained optimization problem

In certain engineering cases, both of the objective function  $f(\mathbf{x})$  and the constraints  $g(\mathbf{x})$  and  $h(\mathbf{x})$  may depend on expensive analysis models. In this subsection, SEO-SRBF for optimization problems with expensive constraints is presented. Incorporated with augmented Lagrangian multiplier method, SEO-SRBF converts a constrained expensive problem into an equivalent unconstrained optimization problem whose expensive augmented Lagrangian function is approximated by RBF. During the optimization procedure, the RBF surrogate of augmented Lagrangian function is gradually upgraded in terms of the increased samples until both of the constraints and the convergence criterion are satisfied. Fig. 3 shows the flowchart of the proposed constrained SEO-SRBF method, which are detailed as follows.

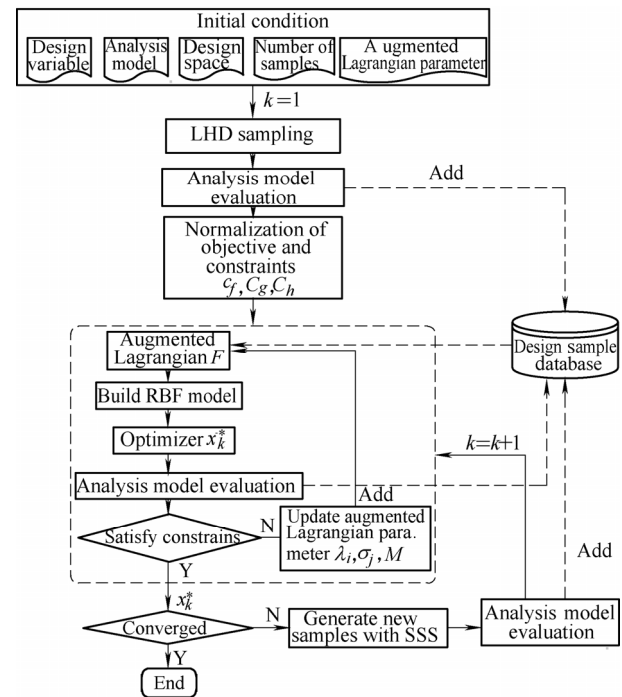


Fig. 3. Flowchart of constrained SEO-SRBF for optimization problems with expensive constraints

Step 1. Initial conditions are configured, such as Lagrangian multipliers  $\lambda_i$  and  $\sigma_j$  for inequal and equal constraints respectively, and the penalty factor  $M$  and the upper bound of the penalty factor  $M_{\max}$ .

Step 2. The initial samples are generated in the entire design space by using LHD, and then the responses at those samples are calculated by calling expensive objective and

constraints respectively. The initial samples and corresponding responses including objective and constraints are stored in the design sample database to construct RBF of augmented Lagrangian function.

Step 3. The normalization parameters in Eq. (11) are evaluated for the objective function and constraints, which is used to normalize the objective and constraints at the aim of improving the convergence property:

$$\begin{cases} c_f = \sum_{s=1}^{N_{\text{initial}}} |f_s| / N_{\text{initial}}, \\ C_{gi} = \sum_{s=1}^{N_{\text{initial}}} |g_{si}| / N_{\text{initial}} \quad (i = 1, 2, \dots, l), \\ C_{hj} = \sum_{s=1}^{N_{\text{initial}}} |h_{sj}| / N_{\text{initial}} \quad (j = 1, 2, \dots, m). \end{cases} \quad (11)$$

Step 4. The objective function and constraints are combined to create the augmented Lagrangian function as shown in Eq. (12):

$$F(\mathbf{x}) = y(\mathbf{x}) + \sum_{i=1}^l [\lambda_i \psi_i + M \psi_i^2] + \sum_{j=1}^m \left\{ \sigma_j u_j(\mathbf{x}) + M [u_j(\mathbf{x})]^2 \right\}, \quad (12)$$

where

$$\begin{cases} \psi_i = \max \left[ p_i(\mathbf{x}), -\frac{\lambda_i}{2M} \right], \\ y(\mathbf{x}) = \frac{f(\mathbf{x})}{c_f}, \\ p_i(\mathbf{x}) = \frac{g_i(\mathbf{x})}{C_{gi}}, \\ u_j(\mathbf{x}) = \frac{h_j(\mathbf{x})}{C_{hj}}, \end{cases} \quad (13)$$

$y$ ,  $p_i$  and  $u_j$  are respectively the normalized responses of objective and constraints. The values of augmented Lagrangian function at the samples in the design samples database can be calculated, and then RBF is constructed to approximate augmented Lagrangian function

Step 5. The potential optimum  $\mathbf{x}_k^*$  is obtained by using GA. Next, the responses at the potential optimum are evaluated by invoking the expensive objective and constraints, which are also added to the samples database.

Step 6. If current potential optimum satisfies all the constraints, the process turns to step 8, otherwise, go to Step 7.

Step 7. Update the augmented Lagrangian multipliers by Eq. (14), then the process returns to step 4. In this work, set the constant  $\alpha=2$  and the upper bound of magnification factor  $M_{\text{max}}=1000$ .

Step 8. Termination criterion in section 2.5 is employed to check whether the optimization converges. If the

termination criterion is met, SEO-SRBF is terminated and outputs the current potential optimum. Otherwise, the process goes to step 9.

$$\begin{cases} \lambda_i^{l+1} = \lambda_i^l + 2M_l \left\{ \max \left[ p_i(\mathbf{x}), -\frac{\lambda_i^l}{2M_l} \right] \right\} \quad (i = 1, 2, \dots, l), \\ \sigma_j^{l+1} = \sigma_j^l + 2M_l u_j(\mathbf{x}) \quad (j = 1, 2, \dots, m), \\ M_{l+1} = \alpha M_l \quad (M_l < M_{\text{max}}), \\ M_{l+1} = M_{\text{max}} \quad (M_l \geq M_{\text{max}}). \end{cases} \quad (14)$$

Step 9. SSS method is used to generate new samples, and then response of expensive objective and constraints are collected. The new samples and corresponding responses are stored in the design samples database. Next, the process goes back to step 4.

### 2.7 Analysis of variable study of SSS method

As discussed in section 2.4, two parameters(i.e.,  $N_{\text{initial}}$  and  $N_{\text{add}}$ ) are required to tune SSS. To assess the sensitivity of the two parameters, the analysis of variance(ANOVA) study on the BR function is carried out in this section. Each parameter has three levels, and the values of each parameter are listed in Table 2. Ten runs are performed for each setting. The total number of function evaluations and the optimal solution are the output in each run, and then, the average values in ten runs of each setting are used for ANOVA study. The ANOVA results including the mean squares and  $p$  value with 95% confidence are listed in Table 3. Fig. 4 and Fig. 5 show the parameter interactions(nfe: number of function evaluations).

Table 2. Variables for ANOVA study

Factor	No. level	Value
$N_{\text{initial}}$	3	3, 6, 12
$N_{\text{add}}$	3	2, 4, 8

Table 3. ANOVA results for parameters

Source	Mean square		$p$	
	Func. Eval.	Func. Opt.	Func. Eval.	Func. Opt.
$N_{\text{initial}}$	61.220	0.295	0.000	0.000
$N_{\text{add}}$	258.040	0.366	0.000	0.000
$N_{\text{initial}} \times N_{\text{add}}$	0.548	0.218	0.000	0.000

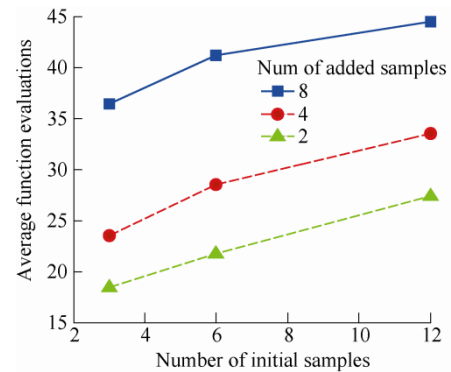


Fig. 4 Parameter interaction plot of average nfe



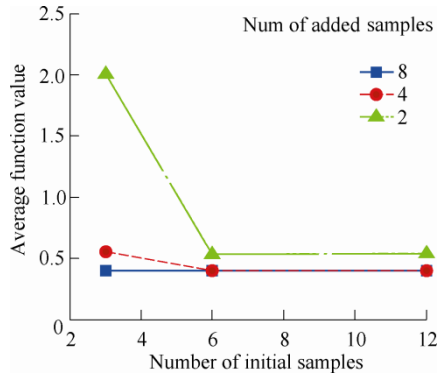


Fig. 5 Parameter interaction plot of average solved optimum

As can be found in Table 3, the number of newly-added samples  $N_{add}$  is more sensitive with respect to both nfe and optimal solution compared with the number of initial samples  $N_{initial}$ . When the number of newly-added samples increases, the number of total samples increase and the approximation accuracy of RBF becomes higher, which leads the process to reach the global optimum. To reduce the computation cost, smaller parameter  $N_{add}$  is suggested (e.g.,  $N_{add}=4$ ). However, if  $N_{add}$  is too small, the SEO-SRBF might miss the true global optimum. From Fig. 5, five pairs of  $N_{initial}$  and  $N_{add}$  obtain the true global optimum of BR. Among those settings, the least computation cost is achieved when  $N_{initial}$  is set to 6 and  $N_{add}$  is set to 4, as shown in Fig. 4. Although the parameter study is conducted on BR function, it is helpful to identify the sensitivity of different parameters, and provides a guideline of parameter setting for numerical examples and engineering applications.

### 3 Numerical and Engineering Examples

In this section, SEO-SRBF is tested on several numerical benchmark problems and two practical engineering design problems. And the optimization results are compared with those from static RBF based optimization, IARSM-II<sup>[20]</sup>, EGO<sup>[14]</sup>, MPPIEGO<sup>[43]</sup>, MSEGO<sup>[44]</sup> and MPS<sup>[25]</sup> to show the merits of SEO-SRBF. The setup of SEO-SRBF in this study is given as follows: 1) LHD method provided by *lhsdesign* function in MATLAB with “*maximin*” criterion (150 iterations) is used for sampling; 2) The multiquadratic function with better accuracy and moderate cost<sup>[3]</sup> is selected as the basis function to build RBF; 3) Due to good capability of searching global optimum<sup>[7]</sup>, GA implemented by *ga* function in MATLAB is employed in RBF surrogate based optimization.

#### 3.1 Numerical examples with SEO-SRBF

SEO-SRBF method is tested on several well-known numerical benchmark problems, and the formulations of them are listed in the Appendix. In this work, the parameters of SEO-SRBF were set as  $[N_{initial}, N_{add}]=[6, 4]$  for low dimension problems (the number of variables is less than 3). For the other problems, the parameters were

set as  $N_{initial}=5n_v$  and  $N_{add}=n_v$ .

The computational cost of SEO-SRBF consists of expensive function evaluations and algorithm execution overhead. All the numerical examples were run on a PC with an Intel Core 2 processor(2.66 GHz), and 5 seconds delay was imposed in invoking each numerical function to measure the time for executing SEO-SRBF.

For each problem, ten runs were performed to reduce random variation in the numerical results and validate the robustness of proposed method. The minimum and the maximum of optimization results were recorded for ten runs, and the median values of optimization results were also reported. To indicate the computation cost, the average CPU time of SEO-SRBF and number of function evaluations were reported. Table 4 shows the average computational cost of ten runs on all the numerical examples. In numerical examples, the average computation cost of SEO-SRBF is less than 1.5% of that for calling functions. In other words, compared with running expensive functions, the algorithm execution time of SEO-SRBF can be totally ignored. Thus, for computation-intensive design optimization problem, computation cost using SEO-SRBF is mainly determined by the number of function evaluations. Similar conclusion has also been given by WANG and SIMPSON<sup>[23]</sup>.

Table 4. Computational cost of SEO-SRBF

Func.	Avg. No. of func. eval.	Avg. CPU time $t/s$		
		Total	Obj.	Algorithm
BR	28.5	144.3	142.5	1.8
RS	44.5	225.4	222.5	2.9
SC	31.5	159.3	157.5	1.8
HN	35.6	179.8	178	1.8

The algorithm overhead of SEO-SRBF was also compared with that of other methods including EGO<sup>[14]</sup>, MPPIEGO<sup>[43]</sup>, MSEGO<sup>[44]</sup> and MPS<sup>[25]</sup>. For a fair comparison, two stopping criteria were provided for EGO, MPPIEGO and MSEGO. Optimization process stopped once the theoretical global optima were found, or maximum number of cycles reached. The number of initial samples of EGO-like methods equals to that of SEO-SRBF for higher dimensional problems, and the maximum number of cycles is set to 50. Ten runs of MPS are performed on each numerical functions. However, since EGO, MPPIEGO and MSEGO are rather time-consuming for solving the high dimensional problems, those methods are performed only once on high dimensional cases. Table 5 and Table 6 summaries the computational cost of the various methods. From comparison of algorithm running time in Table 4 and Table 6, SEO-SRBF is most efficient on all the benchmarks. One possible explanation for that result is that EGO, MPPIEGO and MSEGO employs global optimization subroutines for maximizing the expected improvement to increase samples, which is more time-consuming especially for high dimensional problems. Whereas, SEO-SRBF

directly generates sequential samples in the signification sampling space. Another possible reason for the high efficiency of SEO-SRBF is use of different stopping criteria. SEO-SRBF terminates once the relative error between last two potential optima satisfies the tolerance. In contrast, EGO, MPPIEGO and MSEGO set the maximum number of cycles as stopping criterion, if global optimum can not be obtained within the maximum cycles. Besides, MPS needs to produce a large number of cheap samples to calculate the cumulative probability distribution function for discriminatively sampling, which is still more time-consuming than SEO-SRBF.

**Table 5. Number of function evaluations for different methods**

Func.	EGO	MPPIEGO	MSEGO	MPS
BR	50	102	42	33
SC	42	18	27	30
HN	56	180	180	441
F16	230	230	230	1385

**Table 6. CPU Time for executing different methods(s)**

Func.	EGO	MPPIEGO	MSEGO	MPS
BR	139	1622	32	5
SC	109	76	21	4
HN	233	7217	472	63
F16	416	20568	978	149

Those benchmark functions have been solved by IARSM<sup>[20]</sup>. The comparisons of optimization results on all numerical examples are summarized in Table 7 and Table 8. The first column in Table 7 shows the name of the test function and the theoretical global optimal solutions are given in the third column. As can be seen, the solutions obtained by using SEO-SRBF is better than those from other techniques for each problem. Since the computational expense of RBF surrogate based optimization is negligible compared with that for running expensive functions, the number of function evaluations was used as the indicator of optimization efficiency. Fig. 6 shows a comparison of number of function evaluations of different methods, where y-coordinate indicates the percentages with respect to maximum average number of function evaluations in 10 runs. From Fig. 6, SEO-SRBF uses fewer nfe compared with those of other methods for BR and F16. In addition, the higher efficiency of EGO, MPPIEGO and MSEGO on SC and HN is achieved due to the unfair termination criterion. The true global optima are priori told those method, and once one point close to the true global optimum is found, optimization process is terminated immediately. Whereas, without any priori information on the analytical global optimal solutions, even when current potential optimum gets very close to the true global optimum, SEO-SRBF may still continue to iterate until the tolerance termination criterion is met. In fact, for general engineering applications, it is impossible for designers to know the true global optimum *a priori*, which makes the

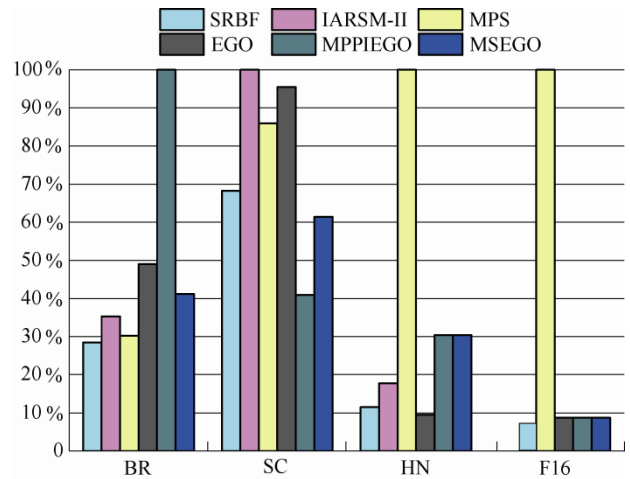
unfair termination criterion of EGO, MPPIEGO and MSEGO no sense for practice. Moreover, the original termination criterion on maximum iteration cycles for EGO-like methods is quite ineffective and inefficient. Thus, the proposed SEO-SRBF is believed to be more efficient than EGO-like methods for real-world applications. Moreover, for HN, the function evaluations for SEO-SRBF are still comparable to the best results. Furthermore, for SC, SEO-SRBF obtains better solutions compared with those of MPPIEGO. Note that for F16 SEO-SRBF shows much better performance on optimization efficiency in comparison with those of other competitors.

**Table 7. Summary of optimal solutions obtained by using SEO-SRBF**

Func.	# of var.	Anal. solu.	Optimal solution	
			Range of variation	Median
BR	2	0.398	[0.398, 0.399]	0.398
SC	2	-1.032	[-1.032, -1.004]	-1.030
HN	6	-3.320	[-3.305, -2.857]	-3.248
F16	16	25.875	[26.260, 27.850]	26.890

**Table 8. Summary of optimal solutions obtained by using other methods (N/A: not available)**

Func.	IARSM-II	MPS	EGO	MPPIEGO	MSEGO
BR	0.398	0.399	0.398	0.418	0.406
SC	-1.029	-1.030	-1.031	-1.027	-1.024
HN	-2.456	-3.305	-3.318	-3.028	-2.400
F16	N/A	27.969	33.200	35.300	27.920



**Fig. 6** Number of function evaluations of various methods on numerical examples

Through the tests on numerical optimization problems above, SEO-SRBF shows the satisfactory performance in both optimization efficiency and global convergence capability. The solutions are generally robust. Note that since all the samples are independent, the CPU time required for running SEO-SRBF can be further reduced by using parallel computation technologies.

### 3.2 Engineering examples with SEO-SRBF

Two engineering design problems were used to validate SEO-SRBF: 1) an internal combustion engineering design



problem, and 2) a torque arm design problem. The latter is a constrained optimization problem involving expensive constraints. For each problem, ten runs were carried out by using the SEO-SRBF and static RBF based optimization method (named Static-RBF), respectively. For the engineering optimization problems, the parameters of augmented Lagrangian are set as  $\lambda_i^1 = 1$ ,  $\sigma_j^1 = 1$ ,  $M_1 = 1$ ,  $\alpha = 2$  and  $M_{\max} = 1000$ .

### 3.2.1 Internal combustion engine design

The internal combustion engine design problem as shown in Fig. 7, was introduced by the Ford Motor Corporation, and was also solved by GANO, et al<sup>[17]</sup>. The objective of the optimization is to maximize the specific power under the packaging and efficiency constraints. The design variables consist of the cylinder bore  $b$ , the compression ratio  $c_r$ , exhaust valve diameter  $d_E$ , intake valve diameter  $d_I$ , and the revolutions per minute at peak power  $w \times 1000$ . The problem is formulated as in Eq. (15).

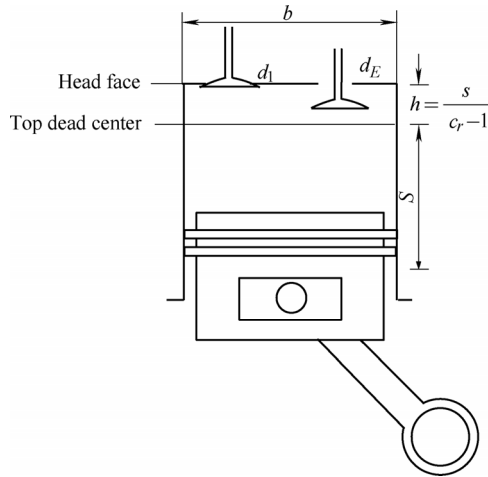


Fig. 7. Illustration of internal combustion engine

$$\max f = K_0((\rho Q / A_f)\eta_t\eta_v - FMEP),$$

where

$$\eta_v = \eta_{vb} [1 + 5.96 \times 10^{-3} w^2] / [1 + [(9.428 \times 10^{-5}) \times (4V / \pi N_c C_s)(w / d_1^2)]^2],$$

$$\eta_{vb} = \begin{cases} 1.067 - 0.038 \exp(w - 5.25) & (w \geq 5.25) \\ 0.637 + 0.13w - 0.014w^2 + 0.00066w^3 & (w \leq 5.25) \end{cases}$$

$$\eta_t = \eta_{tad} - S_v(1.5 / w)^{0.5}$$

$$S_v = 0.83[(8 + 4c_r) + 1.5(c_r - 1)(\pi N_c / V)b^3] / [(2 + c_r)b],$$

$$FMEP = 4.826(c_r - 9.2) + (7.97 + 0.253V_p + 9.7(10^{-6})V_p^2)$$

$$V_p = (8V / \pi N_c)wb^{-2}$$

s.t.

$$g_1 = K_1 N_c b - L_1 \leq 0,$$

$$g_2 = (4K_2 V / \pi N_c L_2)^{1/2} - b \leq 0,$$

$$g_3 = d_1 + d_E - K_3 b \leq 0,$$

$$g_4 = K_4 d_1 - d_E \leq 0,$$

$$g_5 = d_E - K_5 d_1 \leq 0,$$

$$g_6 = (9.428 \times 10^{-5})(4V / \pi N_c)(w / d_1^2) - K_6 C_s \leq 0,$$

$$g_7 = c_r - 13.2 + 0.045b \leq 0,$$

$$g_8 = w - K_7 \leq 0,$$

$$g_9 = 3.6 \times 10^6 - K_8 Q \eta_{tw} \leq 0,$$

$$\eta_{tw} = 0.8595(1 - c_r^{-0.33}) - S_v,$$

(15)

the bounds of design variables are given as  $70 \leq b \leq 90$ ;  $6 \leq c_r \leq 10$ ;  $30 \leq d_E \leq 40$ ;  $35 \leq d_1 \leq 45$ ; and  $4 \leq w \leq 8$ .

The analytical optimum for this engineering problem is 55.67<sup>[17]</sup>. SEO-SRBF was applied to solve this problem 10 times. To indicate the efficiency of SEO-SRBF, the static-RBF based on augmented Lagrangian multiplier method was also used to optimize this problem. The number of initial samples of static-RBF equals to the mean value of nfe of SEO-SRBF. Table 9 summarizes optimization solutions obtained by using SEO-SRBF and static-RBF methods. The initial parameters of SEO-SRBF are set as follows,  $[N_{\text{initial}}, N_{\text{add}}] = [35, 6]$ . As can be seen from Table 9, the best and median values obtained by our proposed SEO-SRBF method are much closer to the theoretical optimum. Moreover, the SEO-SRBF exhibits a superior performance to static-RBF in terms of optimization efficiency. Although static-RBF uses more samples uniformly distributed in the entire design space, the optimum solution is still inferior to that of SEO-SRBF.

Table 9. Optimization solutions of internal combustion engine design problem

Method	Objective value		No. of obj. eval.	
	Best	Median	Mean	Median
SEO-SRBF	54.47	51.40	140	102
Static-RBF	53.69	47.98	162.9	162.5

### 3.2.2 Torque arm design

A torque arm (shown in Fig. 8), typical mechanical part in mechanical engineering, was selected to test SEO-SRBF. The objective of this design problem is to minimize the volume of material subject to the maximum stress constraint (i.e., less than 190 MPa).

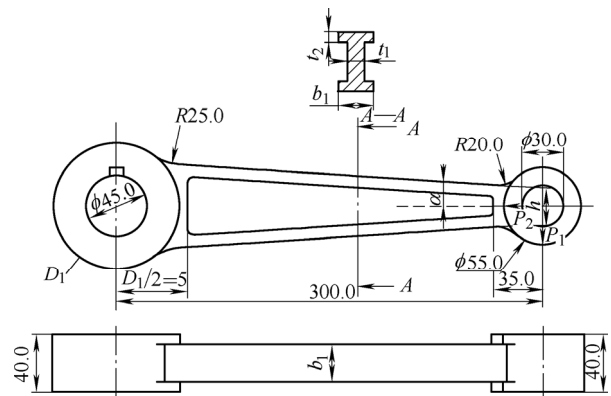


Fig. 8 Geometry and parameterization of torque arm

The force  $P_1 = 8$  kN and  $P_2 = 4$  kN act at the center of the smaller end. The boundary condition is that the torque

arm is fixed at the hole of the bigger end. Young's modulus and Poisson's ratio are 200 GPa and 0.3 respectively. This problem involves six design variables  $\alpha, b_1, D_1, h, t_1$  and  $t_2$  as depicted in Fig. 8, and the design space is defined as follows,  $3.0 \leq \alpha \leq 4.5$  ( $^\circ$ ),  $25.0 \leq b_1 \leq 35.0$  (mm),  $90.0 \leq D_1 \leq 120.0$  (mm),  $20.0 \leq h \leq 30.0$  (mm),  $12.0 \leq t_1 \leq 22.0$  (mm) and  $8.0 \leq t_2 \leq 10.0$  (mm).

In this problem, UG and MSC.Patran/Nastran were used to build an automatic integration system for solving this torque arm optimization through script programming. The problem is a nonlinear constrained problem involving computation-intensive objective and constraint, and thus reduction of expensive analysis model evaluations is our concern. The SEO-SRBF method and static-RBF based on augmented Lagrangian method were applied to solve this problem. The number of initial samples of static-RBF equals to the number of model evaluations needed by SEO-SRBF.

Table 10 shows the comparative results between SEO-SRBF and static-RBF. It can be seen that the number of model evaluations required by SEO-SRBF is the same as that of static-RBF. However, SEO-SRBF further reduces 21% of the material volume of torque arm compared with static-RBF. But for Static-RBF, some more samples are needed to get a comparable result. The results shows that the computation cost can be reduced by SEO-SRBF for real-world engineering optimization problems with expensive objective and constraints. Fig. 9 shows the iteration history of the objective in the course of SEO-SRBF optimization process. Fig. 10 depicts the shape and stress contour of the optimal design obtained by using SEO-SRBF. The optimum shape results in the more uniform stress distribution in the body of the torque arm.

**Table 10. Optimization results of torque arm design problem**

Method	Optimum [ $\alpha, b_1, D_1, h, t_1, t_2$ ]	Volume $V/\text{cm}^3$	Stress $S/\text{MPa}$	No. of model eval.
SEO-SRBF	[4.25, 27.22, 90.00, 24.38, 12.75, 8.24]	455	173	80
Static-RBF	[4.02, 30.28, 97.58, 29.08, 19.97, 9.55]	576	128	80

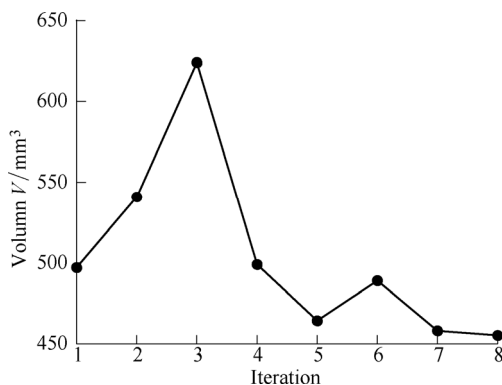


Fig. 9 Objective iteration history of torque arm optimization by using SEO-SRBF

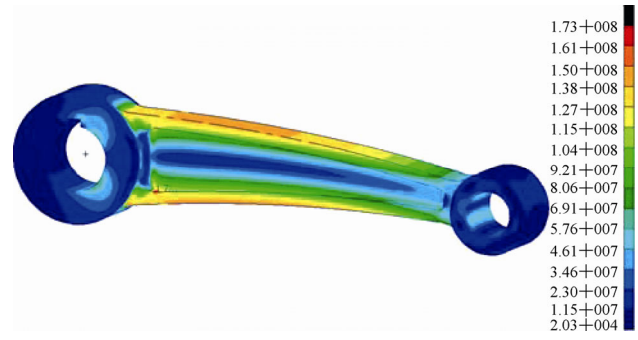


Fig. 10 Stress contour of optimal design of torque arm obtained by using SEO-SRBF

### 4 Discussion

For engineering design optimization problems, designers usually desires to reach the actual global optimum with the least computational burden. The proposed SEO-SRBF features the high optimization efficiency and good capability of searching true global optima by using significant sampling space(SSS) method. Fig. 11 details the sampling and optimization process of SEO-SRBF is illustrated on Branin function(BR) to reveal the characteristics of SEO-SRBF and SSS method.

In Fig. 11, the green square and black points indicate the true global optimum (3.141 5, 2.274 9) and design samples respectively, and red rhombus points represent the potential optima during the optimization procedure. Twenty-two function evaluations are required by SEO-SRBF to optimize BR. From Fig. 11, it can be observed that the SEO-SRBF has the following three properties: 1) It can converge to the true global optimum of BR; 2) More sequential samples trends to concentrate around the true global optimum of BR as iteration continues; 3) The potential optima gradually approach to the true global optimum and finally almost overlaps with it at the last iteration.

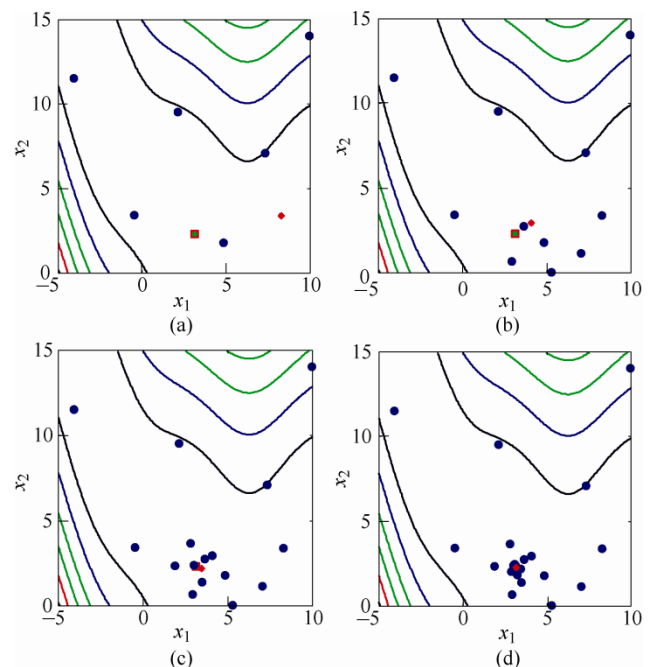


Fig. 11 Optimization process of SEO-SRBF on BR

Fig. 12 shows the graphics of BR and RBF surrogates from SEO-SRBF and Static-RBF in the entire design space. Twenty-two evenly distributed samples in the entire design space are used to build static RBF. Although global approximation accuracy of static RBF is apparently much better than that of SEO-SRBF, both RBF surrogates cannot well approximate the true BR in the entire design space. Fig. 13 depicts the contours of BR and RBF surrogates in the neighborhood of the true global optimum. From Fig. 13, it can be seen that the contours SEO-SRBF are almost identical with those of BR around the global optimum, which is much better than static RBF. During SEO-SRBF optimization process, all of the new sequential samples are positioned in relative small region towards the true global optimum, whereas for static RBF, plenty of samples are wasted in the unconcerned regions far from the true global optimum.

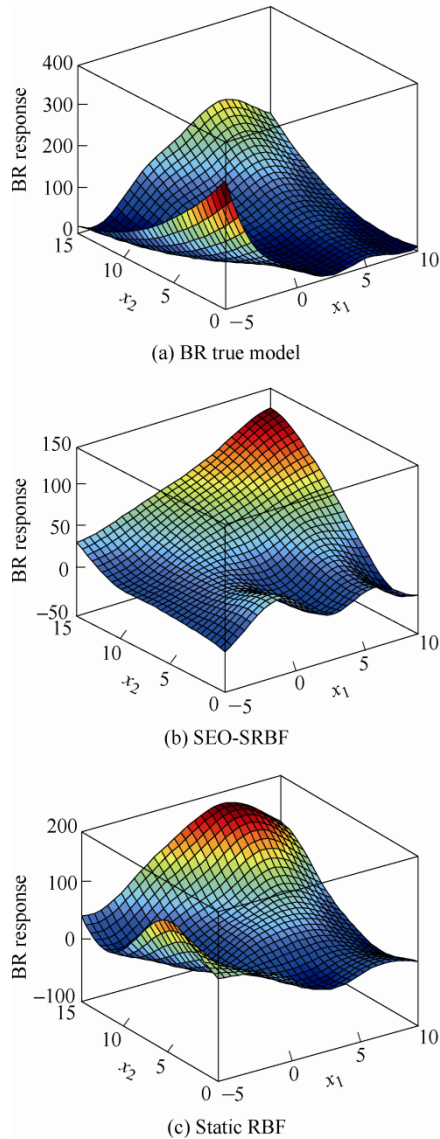


Fig. 12 Graphics of BR and RBF surrogates in entire design space

One challenge for RBF modeling is that matrix  $A_r$  might become ill-condition or even singular when samples get very close to some others. In this case, the fitting problem

usually appears difficulties in calculating  $A_r^{-1}$ . For that issue, the method proposed by JONES, et al<sup>[14]</sup>, was used to conduct singular value decomposition of  $R$  when huge condition number of  $A_r$  appears.

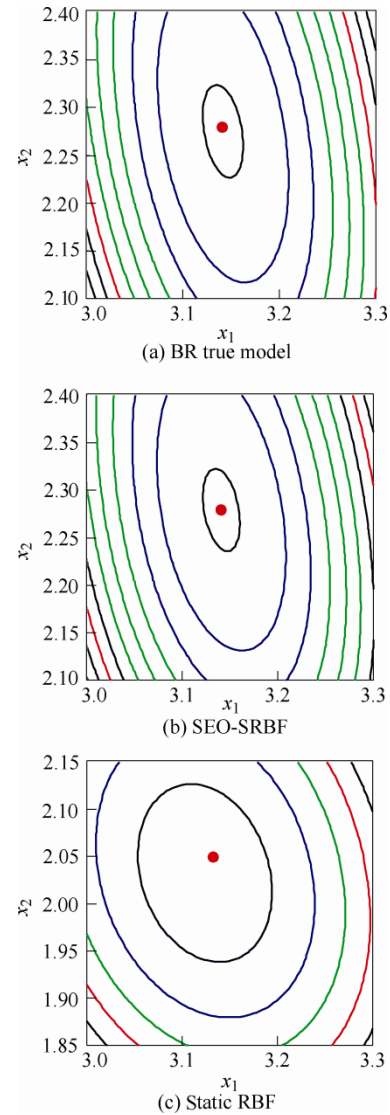


Fig. 13 Contours of BR and RBF surrogates in the neighborhood of true global optimum

## 5 Conclusions

(1) A novel surrogate-based efficient optimization method using sequential radial basis function, notated as SEO-SRBF is proposed for constrained expensive engineering optimizations. SSS method is developed to generated sequential samples towards the global optimum for updating RBF surrogate.

(2) For constrained optimization problems, SEO-SRBF employs the augmented Lagrangian multiplier method to handle expensive constraints.

(3) Through several numerical benchmark problems and two engineering problems, SEO-SRBF is compared with some other optimization methods including static RBF based optimization, IARSM-II, EGO, MPPIEGO, MSEGO and MPS. The comparison results demonstrate that

SEO-SRBF exhibits satisfactory performance in optimization efficiency, global convergence capability, and robustness.

(4) The sequential sampling and optimization process are visually illustrated on a two dimensional problem to discuss the features of SEO-SRBF.

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