Journal of Mechanical Science and Technology

Journal of Mechanical Science and Technology 23 (2009) 2903~2912

www.springerlink.com/content/1738-494x DOI 10.1007/s12206-009-0806-5

A response surface based sequential approximate optimization using constraint-shifting analogy[†]

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(Manuscript Received February 12, 2009; Revised July 2, 2009; Accepted July 25, 2009)

Abstract

When a traditional response surface method (RSM) is used as a meta-model for inequality constraint functions, an approximate optimal solution is sometimes actually infeasible in a case where it is active at the constraint boundary. The paper proposes a new RSM that ensures the constraint feasibility with respect to an approximate optimal solution. Constraint-shifting is suggested in order to secure the constraint feasibility during the sequential approximate optimization process. A central composite design is used as a tool for design of experiments. The proposed approach is verified through a mathematical function problem and engineering optimization problems to support the proposed strategies.

Keywords: Sequential approximate optimization; Response surface method; Constraint feasibility; Constraint-shifting analogy

1. Introduction

The response surface method (RSM) [1] has been recognized as one of the most efficient approximation tools in the context of sequential approximate optimization (SAO). There has recently been considerable attention given to RSM based approximation optimization in areas of mechanical and aerospace design optimization [2-7]. RSM is also an efficient approach that contributes to the probabilistic design such as robust and/or reliability-based design optimization [8, 9].

A special care should be taken when RSM is used as a function approximation tool in the inequalityconstrained optimization problems. Given a number of known input-output training data generated from design of experiments (DOE), a well-trained RSM <u>can be obtained by the least square method that</u> [†]This paper was recommended for publication in revised form by minimizes the absolute difference between actual outputs and approximate outputs, normally formulated in terms of mean squared error. A conventional RSM shows the approximation result such that an actual output may be larger or smaller than its corresponding approximate value due to the implementation of 'absolute difference' or 'mean squared error' between them. In approximate optimization problems, the objective function and equality/inequality constraints would be described using RSM-based metamodels. A conventional version of RSM can be simply applied to the meta-modeling of an objective function since the minimized or maximized solution would be obtained according to the extent of its metamodeling accuracy. However for nonlinear inequality constraints, when the optimal design by approximate optimization is found on the active constraint boundary, such design is most likely to be actually infeasible [10, 11]. The advantage of employing metamodels in the approximate optimization is to obtain the reliable design solutions in addition to savings in computational costs. One can easily expect that the

Associate Editor Tae Hee Lee

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meta-models have an ability to replace the expensive engineering analysis, but its approximate optimal solutions may not be accepted if they are actually infeasible. It should be noted that the design solution should be at least satisfied with design constraint rather than simply and solely minimizing or maximizing the objective function value.

The present study deals with how efficiently usable and feasible design solutions are found in the context of RSM-based sequential approximate optimization. The paper suggests a new RSM-based meta-model that enhances the constraint feasibility with respect to approximate optimal solution. The trust region management scheme and a number of convergence conditions [12, 13] are adopted in the present study. The trust management scheme is developed by using the pattern search algorithm, and such concept is explored to unconstrained optimization problems in order to secure the global convergence [14, 15]. The augmented Lagrangian method facilitates solving constrained problems in the context of sequential response surface approximation and optimization [12]. The interior-point method is implemented to ensure the approximation feasibility [13]. The moving least square method is introduced in RSM [16]. However, such methods require computationally expensive sensitivity information, and do not verify the constraint feasibility about the approximate optimum.

In the present study a constraint-shifting (CS) is proposed in order to secure the constraint feasibility during the RSM-based SAO process. Such strategy is analogous to the shifting constraint method used in the robust optimization [17, 18]. The present approach is verified through a constrained mathematical function problem and a number of engineering optimization problems in order to support the proposed strategies.

2. Response surface method

The response surface has a model of the form [3];

$$y(x) = f(x) + \varepsilon \tag{1}$$

where, y(x) is the unknown function of interest, f(x) is a known polynomial function in terms of x, and ε is a random error that is assumed to be normally distributed with mean zero and variance σ^2 . The polynomial function, f(x) to approximate, y(x) is typically chosen as a 2nd order polynomial in order to accom-

modate the nonlinearity in the model as follows:

$$f(x) = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_i \sum_{j>i} \beta_{ij} x_i x_j$$
(2)

where, *k* is the number of design variables. The parameters of β_{ij} are determined via the least square method which minimizes the squared sum of the deviations of predicted values, *f*(*x*) from the actual values, *y*(*x*). Such parameters can be obtained byg the following relation:

$$\tilde{\beta} = [\bar{X}^T \bar{X}]^{-1} \bar{X}^T \tilde{y} \tag{3}$$

where, \overline{X} is the design matrix calculated from training data, and \tilde{y} is a column vector containing the values of the response at each training data.

3. Design of experiments

A number of training data are required to generate the response surface for a function with n design variables. It is important to employ an efficient quantity and distribution of training data over the design space of interest. In the present study, response surfaces are obtained based on the central composite design (CCD) in the context of design of experiments (DOE). The CCD in the computer experiments uses a total of $2^n + 2n + 1$ training data, where *n* is the number of design variables. The CCD consists of two-level factorial, the corner points of a hypercube together with the center point and star points arranged along the axes of the variables and symmetrically positioned with respect to the factorial hypercube [12]. It is noted that the CCD requires a lower number of design points than the full factorial design. Even though, for the large dimensionality design problem, the CCD becomes unsatisfied, the present study adopts the CCD to present the constraint feasibility in constructing the RSM.

4. Inequality constraints

Suppose there is a 2nd order polynomial with coefficients, β_{ij} . For a total of *L* training DOE data, an RSM can be obtained by minimizing the absolute difference between actual outputs and approximate outputs as follows:

Find
$$\beta_{ij}$$
 (4)

Minimize
$$E = \frac{1}{2} \sum_{l=1}^{L} (g_{actual,l} - g_{RSM,l}(\beta_{ij}))^2$$
 (5)

where, $g_{actual,l}$ and $g_{RSM,l}$ are actual and RSM (approximate) output values of a response (i.e., constraint function), respectively. The result of Eqn. (4) is the least square method based response surface as shown in Eqn. (3). The general expression for a nonlinear inequality constraint, *g* can be typically written as follows:

$$p_{lower} \le g \le p_{upper} \tag{6}$$

where p_{lower} and p_{upper} are problem parameters, normally constant values that limit lower and upper bounds on constraint, respectively. The discrepancy between actual and approximate constraint values in Eqn. (5) can be shown in Fig. 1(a), where the violation of constraint feasibility is detected at some approximate points so that the approximate optimal design x_a^* would happen to be actually infeasible as shown in Fig. 1(b) of Reference [10]. Thus, the least square method for RSM would be modified by adding two constraint conditions as follows:

Minimize
$$E = \frac{1}{2} \sum_{l=1}^{L} (g_{actual,l} - g_{RSM,l}(\beta_{ij}))^2$$
 (7)

subject to
$$g_{actual,l} - g_{RSM,l}(\beta_{ij}) \le 0$$

for
$$(g_{actual,l}(\beta_{ij}) \ge p_{upper})$$
 (8)

$$g_{actual,l} - g_{RSM,l}(\beta_{ij}) \ge 0$$

$$\text{for } (g_{actual,l}(\beta_{ij}) \le p_{lower})$$

$$(9)$$

A new condition for the upper limit, Eqn. (8) is introduced such that the *l*-th approximate output $g_{RSM,l}$ should be greater than or equal to the *l*-th actual output $g_{actual,l}$ in a case where $g_{actual,l}$ is greater than or equal to p_{upper} , implying that by making such approximate output infeasible, this is not selected during the optimization process. It is noted that the optimal solution is determined by approximate value, not actual value in the context of sequential approximation optimization. The feasibility of an actual output could be also guaranteed in a case where an approximate output is the same as the upper limit of p_{upper} . That is, when the approximate optimal solution is obtained on the constraint boundary (i.e., the constraint is active), its corresponding actual design is always less than or equal to the upper limit,



(a) Some approximate designs would be actually infeasible, not active



(b) An approximate optimal design x_a^{*} is actually infeasible

Fig. 1. Constraint violation of approximate optimum cited from Ref [10].

resulting in the constraint feasibility. This approach is said to be a conservative approximation in terms of actual output and approximate output; a formulation definitely pushes the unfavorable approximate value (i.e., inside of shaded area in Fig. 1(a)) into the infeasible region [10]. Eqn. (9) for a lower limit is also applied so that the infeasible approximate output below p_{lower} is not selected as well.

Conditions of Eqns. (7) to (9) can be formulated by using a sequential unconstrained minimization technique such as exterior penalty function method [11] or Lagrangian multiplier method. However, such formulations require a large number of training data in order to establish an accurate level of constraintconditioned RSM. In a case where the CCD or its similar version of DOE is used, the training result is not good due to their limited number of sampling points so that the alternatives should be employed. The paper proposes an efficient constraint-shifting that helps secure the constraint feasibility during the RSM-based SAO.

5. Constraint-shifting analogy

The concept of constraint-shifting has been for-

merly applied in the context of robust optimization [18]. The shifting constraint method reformulates the robust constraint in terms of the original constraint and their derivatives with respect to design variables within the design tolerance as follows:

$$g_j^{robust} = g_j + \alpha_j \cdot \sum_{i=1}^n \left| \frac{\partial g_j}{\partial x_i} \right| \Delta x_i \le 0$$
(10)

where, α_i is a positive constant that makes the feasible region more tightened, and Δx_i is the tolerance of a design variable. The second term in the right hand side of Eqn. (10) is interpreted as the variation of a constraint within an allowable region of tolerance, describing the robust feasibility.

Instead of the full formulation described in the earlier section, the present study proposes a new constraint-shifting (CS) as follows:

$$g_{RSM-CS} = g_{RSM} + \alpha \cdot \Omega_{upper} \le 0 \tag{11}$$

There is an analogy between Eqns. (9) and (10). The term Ω_{upper} is not necessary when all of the actual constraint values calculated from DOE data are less than the upper bound. For the case where there is more than one DOE data whose actual constraint value is greater than the upper bound (i.e., $g_{actual,l} \ge p_{upper}$) as shown in Figure 2, count the number of such DOE data, denoted by x_m^{CS} , (m = 1, ..., M), where *M* is a total of such counters. The next is to evaluate averages of $g_{actual}(x_m^{cS})$ and $g_{RSM}(x_m^{CS})$. Thus, the added term is written as follows:

$$\Omega_{upper} = \frac{1}{M} |\sum_{m=1}^{M} g_{actual}(x_m^{CS}) - \sum_{m=1}^{M} g_{RSM}(x_m^{CS})|$$
(12)

Likewise, the lower bound case of $g_{actual,l} \le p_{lower}$ is expressed as written below.

$$g_{RSM-CS} = g_{RSM} + \alpha \cdot \Omega_{lower} \le 0 \tag{13}$$

$$\Omega_{lower} = -\frac{1}{M} \left| \sum_{m=1}^{M} g_{actual}(x_m^{CS}) - \sum_{m=1}^{M} g_{RSM}(x_m^{CS}) \right| (14)$$

The value of $\alpha = 1.0$ is used in the present study. It is noted that Eqns. (12) and (14) are quite similar to the second term in the right hand side of Eqn. (10). That is, the variation of a constraint within an allowable region of tolerance is to the robust optimization



Fig. 2. Constraint-shifting for upper bound case.

as the averaged difference between $g_{actual}(x_m^{cS})$ and $g_{RSM}(x_m^{CS})$ within the current DOE space is to the constraint-shifting analogy. A function g_{RSM} is moved to the solid curve of g_{RSM-CS} by the directed amount of Ω_{upper} as shown in Fig. 2. In a case where an approximate optimal solution is obtained at the constraint boundary of the upper bound, and its corresponding actual design would be feasible. Such solid-curves g_{RSM-CS} can be successively moved toward dotted curves when $\alpha > 1.0$ is to be used. The CS analogy makes approximate constraint values conservative, thereby compensating for the constraint feasibility.

6. Trust region management

The constraint-feasible RSM-based SAO is proposed in the present study, wherein the modified version of the trust region management scheme and a number of convergence conditions are adopted from Reference [12]. The steps for the constraint-feasible RSM-based SAO together with trust region management and move limit strategies are discussed in a greater detail for the completeness of the present paper.

During the *k*-th iteration of SAO process, the trust region Γ^k is defined as follows:

$$\Gamma^{k} = \{ x : || x - x_{k} || \le h^{k} \}$$
(15)

where, h^k is referred to as a move limit. The design accuracy between actual objective function value, $f(x_k)$ and approximate objective function value, $\tilde{f}(x_k)$ is evaluated by using ρ^k as follows:

$$\rho^{k} = \frac{\Delta^{k}_{actual}}{\Delta^{k}_{predicted}} = \frac{f(x_{k}^{0}) - f(x_{k}^{*})}{\tilde{f}(x_{k}^{0}) - \tilde{f}(x_{k}^{*})}$$
(16)



Fig. 3. Procedure of response surface based SAO for constraint feasibility.

where, x_k^0 and x_k^* are starting and final approximate designs, respectively, during the *k*-th iteration of SAO. The trust region ratio is controlled via ρ^k in terms of the reduction of approximate optimal objective function value, $\Delta_{predicted}^k$ and the reduction of actual optimal objective function value, Δ_{actual}^k .

Step-1: Initialize the design variable values, and suppose initial values such as move limit control constants, $\gamma_1, \gamma_2, \gamma_3$ and trust region ratio constant, η .

Step-2: Perform the DOE process using CCD.

Step-3: Evaluate the single iteration of the proposed RSM-based SAO for constraint feasibility. It is noted that for example, the constraint-feasible response surface is obtained from Eqns. (11) and/or (13).

Step-4: Calculate the trust region ratio, ρ^k using Eqn. (16).

Step-5: Subsequently, the trust region and the move limit are determined as follows:

Case-1) $\rho^k \leq 0$

This is a case where the approximate objective function value at the approximate optimal design is reduced even though the actual objective function value is not reduced. The design variables are assigned as $x_{k+1} = x_k$ and the move limit is selected as $h^{k+1} = \gamma_1 h^k$ for a new design region.

Case-2)
$$0 < \rho^k < \eta$$
 or $0 < \frac{1}{\rho^k} < \eta$

The predicted reduction $\Delta_{predicted}^{k}$ is more reduced than the actual reduction Δ_{actual}^{k} for $0 < \rho^{k} < \eta$. In this case, design variables are changed as $x_{k+1} = x_{k}^{*}$ and the move limit is also taken as $h^{k+1} = \gamma_{1}h^{k}$.

Case-3)
$$\eta < \rho^k < 1$$
 or $\eta < \frac{1}{\rho^k} < 1$

The actual reduction is quite similar to the predicted reduction so that design variables are assigned as $x_{k+1} = x_k^*$ and the move limit becomes $h^{k+1} = \gamma_2 h^k$.

Case-4) $\rho^k \approx 1$

This is a case where the approximate model is almost the same as the actual value. If $||x_k^* - x_k|| = h^k$, then $h^{k+1} = \gamma_3 h^k$, otherwise, $h^{k+1} = h^k$ and $x_{k+1} = x_k^*$.

Step-6: Go to Step-2, and do the next iteration $(k \rightarrow k+1)$ of SAO until the convergence conditions as written below are satisfied.

$$\rho^k \le \varepsilon_1 \tag{17}$$

$$|f(x_k) - f(x_{k-1})| \le \varepsilon_2 \tag{18}$$

$$\frac{|f(x_k) - f(x_{k-1})|}{\max(|f(x_k)|, \tau)} \le \varepsilon_3$$
(19)

$$\rho^{k} = \rho^{k-1} \text{ and } \frac{|x_{k} - x_{k-1}|}{\max(|x_{k}|, \tau)} \le \varepsilon_{4}$$
(20)

where, τ is the comparison parameter. The SAO is converged when the design region should be less than ε_1 . The convergence condition is also met when the change between the current and previous objective function values should be less than ε_2 . Two more convergence conditions are considered such that the relative rate change of objective function values should be less than ε_3 , and the relative rate change of design variable values between the current and previous truss region should be less than ε_4 . The present study uses a total of four convergence conditions for the termination of the SAO process. The proposed procedure of response surface based SAO for ensuring constraint feasibility is demonstrated in Fig. 3

7. Design applications

The present study explores a constrained function minimization problem and a number of engineering optimization problems. For design applications, the central composite design (CCD) is used in the context of design of experiments. The move limit control values are selected as $\gamma_1 = 0.25$, $\gamma_2 = 0.75$, and $\gamma_3 = 1.25$. The trust region ratio is taken as $\eta = 0.75$. As an optimizer during the SAO process, the method of feasible direction (MFD) is used.

7.1 Mathematical function problem

Consider the following constrained minimization problem:

Minimize
$$f = X_1^2 - 0.5X_2^2$$
 (21)
subject to $g_1 = 0.0372(X_1^2 + X_1X_2 + X_2^2)$
 $-189.5614(X_1^5 - X_2^4) \le 0$
 $g_2 = 0.0017X_1X_2^2$
 $-1.1488(X_1^3 - X_2^3) - 30.3470 \le 0$

The numerical data are obtained through CCD, and sequential approximation optimization is subsequently conducted after the response surface metamodels are established. Results by two RSM methods are compared in Table 1. The 'proposed RSM' (RSM-CS) facilitates to finally provide an actually feasible optimal design while the 'RSM without constraint-shifting' (RSM) does not. The progressive design convergence between actual and approximate constraints under RSM-CS is graphically represented as shown in Fig. 4. Solid lines indicate actual constraints, and dotted lines mean approximate constraints. Feasible regions are located on and under each of the constraint function curves. The objective function contour is not included for the brevity of graphs. These results show that the approximate optimal design is coincident with its corresponding actual optimal design that is absolutely feasible.

7.2 Ten-bar planar truss design

As an example of an engineering design problem, a ten-bar truss optimization in Figure 5 is explored. The design objective is to find cross sectional areas of truss members, X_i (*i*=1, 10) by minimizing the total weight of a structure $W(X_i)$ with stress constraints [19]. The optimization statement is written as follows:

Minimize
$$W(X_i)$$
 (22)
subject to $\sigma_j^{Lower} \le \sigma_j \le \sigma_j^{Upper}$
 $X_i^{lower} \le X_i \le X_i^{upper}$

In this design problem, both RSM and RSM-CS finally produce actually feasible optimal designs with the same number of function evaluations as shown in



Fig. 4. Solution convergence during SAO.

Table 2, wherein a non-approximate optimal design is also compared. Convergence histories of two methods are shown in Figure 6, wherein RSM-CS violates the actual constraints two times in the middle of convergence. In the constraint-shifting analogy, $\alpha = 1.0$ is used in Eqns. (11) and (13). The value of $\alpha > 1.0$ can make an approximate constraint value more feasible, but it results in such contour being much too conservative accompanied with the unexpected increase in objective function value. To maintain the approximate optimal solution as always actually feasible during SAO, an adaptive strategy for α should be implemented. The present study uses a fixed value of $\alpha = 1.0$ for all numerical examples, implying that only Ω_{upper} (or Ω_{lower}) term is considered in constraint-shifting analogy.

7.3 Cylinder spring



Fig. 5. Ten-bar planar truss



Fig. 6. Convergence histories of ten-bar planar truss.



Fig. 7. Convergence histories of cylinder spring design.

The design objective is to determine the coil diameter (d), the cylinder's mean diameter (D) and the number of active coils (N) by minimizing the weight of the cylinder spring subjected to constraints on deflection, shear stress and natural frequency with a geometrical condition [20]. The mathematical statement of this optimization problem is given as follows:

Minimize
$$f = (N+2)Dd^2$$
 (23)
subject to $g_1 = 1.0 - \frac{D^3N}{71875d^4} \le 0$
 $g_2 = \frac{D(4D-d)}{12566d^3(D-d)} + \frac{2.46}{12566d^2} - 1.0 \le 0$
 $g_3 = 1.0 - \frac{140.54d}{D^2N} \le 0$
 $g_4 = \frac{D+d}{1.5} - 1.0 \le 0$
 $0.05 \le d \le 0.20(in)$
 $0.25 \le D \le 1.30(in)$
 $2 \le N \le 15$

where, the number of active coils is treated as continuous design variable in the present study. RSM-CS results in the finally feasible optimal design, while RSM doe not as shown in Table 3, wherein a nonapproximate optimal design by I-Design is presented. The proposed RSM-CS is also better than RSM in terms of the number of function evaluations. Convergence histories of two methods are shown in Figure 7. Even though design solutions are infeasible during the early stages of SAO, the proposed RSM-CS converges with feasible designs after the third SAO iteration.



Fig. 8. Piston design.

7.4 Piston design

The design objective of this problem is to locate the piston components, x_1 , x_2 , x_3 , and D by minimizing the oil volume when the lever of the piston is lifted up from 0deg to 45deg as shown in Fig. 8. The formal optimization statement is given as follows [21]:

Minimize $f(X) = \pi D^2 (b-a)/4$	(24)
subject to $QL\cos 45^o - RF \le 0$	
$Q(L-x_3) - M_{\max} \le 0$	
$1.2(b-a) - a \le 0$	
$D/2 - x_2 \le 0$	
$R = \frac{ -x_3(x_3\sin\theta + x_1) + x_1(x_2 - x_3\cos\theta) }{ }$	
$\sqrt{(x_3 - x_2)^2 + x_1^2}$	

$$F = \pi PD^2 / 4$$

$$a = \sqrt{(x_3 - x_2)^2 + x_1^2}$$

$$b = \sqrt{(x_3 \sin 45^0 + x_1)^2 + (x_2 - x_3 \cos 45^0)^2}$$

$$0.05 \le x_1, x_2, D \le 1,000$$

$$0.05 \le x_3 \le 120$$

where, the payload is Q=10,000lbs, the lever is L=240in in length, the maximum allowable bending moment of the lever is M_{max} =1.8E+06lbs-in, and the oil pressure is given as 1,500psi. A number of inequality constraints are imposed; force equilibrium, maximum bending moment of the lever, minimum piston stroke and geometrical condition are considered.

RSM-CS locates the finally feasible optimal design,



Fig. 9. Convergence histories of piston design.

while RSM converges to the infeasible design as shown in Table 4. Convergence histories of two methods are shown in Figure 9, wherein RSM-CS converges with feasible designs after the third SAO.

Table 1. Results of mathematical function problem.

	Initial design	Direct MFD	RSM	RSM-CS
X1	7.5	5.0	5.0925	5.0
X2	7.5	5.3275	5.4817	5.3155
OBJ	28.125	10.8091	10.9080	10.8278
Final solu- tion	-	feasible	infeasible	feasible
# of SAO iterations	-	-	3	3

Table 2. Results of ten-bar planar truss.

	Initial design	Optimal design [19]	RSM	RSM-CS
X1	5.0	7.90	7.8214	7.9995
X2	5.0	0.10	0.1124	0.1341
X3	5.0	8.10	8.2654	8.1568
X4	5.0	3.90	4.0232	3.9654
X5	5.0	0.10	0.1214	0.1115
X6	5.0	0.10	0.1511	0.1024
X7	5.0	5.80	5.9932	6.1297
X8	5.0	5.51	5.8516	5.6212
X9	5.0	3.68	3.9138	3.8013
X10	5.0	0.14	0.1467	0.1821
OBJ	2098.2	1498.0	1547.6	1537.9
Final solu- tion	-	feasible	feasible	Feasible
# of SAO iterations	-	-	12	12

Table 3. Results of cylinder spring.

	Initial design	I-Design [20]	RSM	RSM-CS
d	1.0	0.0534	0.0518	0.0520
D	2.0	0.3992	0.3585	0.3632
Ν	3.0	9.1854	11.2912	11.0212
OBJ	10.0	0.01273	0.0128	0.0128
Final solu- tion	-	feasible	infeasible	feasible
# of SAO iterations	-	-	8	7

Table 4.	Results	of	piston	design.
		~ ~ !		

	Initial design	RSM	RSM-CS
X1	45.0	50.85	50.91
X2	6.0	3.25	3.27
X3	115.0	120.0	120.0
D	3.0	6.53	6.52
OBJ	206.0	1038.1	1036.4
Final solution	-	infeasible	Feasible
# of SAO iterations	-	6	6

8. Concluding remarks

The paper discusses a new RSM-based approximation that ensures the constraint feasibility in the context of sequential approximate optimization. Approximations of inequality constraint function bounded by both lower and upper limits are considered. It is emphasized that optimal designs obtained from approximate optimization strategies may not be accepted if they are actually infeasible. A constraintshifting analogy is suggested in order to reinforce the constraint feasibility during the RSM based SAO process. The proposed RSM is validated via a mathematical function problem and a number of engineering optimization problems. In design problems, the proposed approach locates an approximate optimum within a feasible design domain, while a conventional RSM sometimes results in the actually infeasible approximate optimal solution. As further research in this context, it would be more valuable to apply proposed approach to other approximation and meta-modeling techniques such as support vector machine and Kriging, etc. when inequality constraints should be carefully taken in the context of sequential constrained approximate optimization.

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