An Improved Surrogate Based Optimization Method for Expensive Black-box Problems

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Abstract. For expensive black-box problems, surrogate modelling techniques are generally used to decrease the computational source. In this study, an improved surrogate based optimization (SBO) method is presented to solve the real-world engineering applications with expensive black-box objective responses. An optimized ensemble of surrogates combing three typical surrogate modelling techniques is adapted to efficiently predict the objective response. Meanwhile, the hierarchical design space reduction (HSR) strategy is employed for obtaining the smaller design subspace for improving the optimization efficiency. During the search, all test problems are considered as the real-world engineering applications whereas the actual global optima as well as the function characteristics are unknown in advance. The results show that the proposed method is superior in identifying the global optimum.

1. Introduction

The rapid progress of the engineering applications like underwater vehicles has improved the significance for optimal design of the related industrial products. Nevertheless, the classical optimization methods like ant colony algorithm, genetic algorithm (GA) generally require plenty of computationally expensive function evaluations to identify the acceptable optima. To overcome the computational difficulty, SBO approaches are broadly employed for accelerating the search process. A new SBO method called SEUMRE is introduced to handle the engineering design optimization problems in literature [1]. A metamodel-based optimization approach named HAM which can adaptive select suitable metamodeling techniques is presented in literature [2]. Shi et al. use the radial basis functions (RBF) method for handling the satellite constellation system problem [3]. Sun et al. use the efficient global optimization (EGO) method to obtain the higher maximum LDR for underwater vehicles [4]. However, these studies remain unclear which surrogate modeling technique is most suitable for a given problem.

To achieve the better optimal results and reducing the number of function evaluations (NFE), ensemble of surrogates has been recently drawn considerable attention and proven a promising method for various optimization problems. Goel et al. present a novel weight factors selection method selected weight factors using a given global error measure [5]. The corresponding weights are calculated by solving an optimization problem in literature [6]. Lee and Choi use the prediction point of interest to obtain the pointwise ensemble of surrogates [7].
Motivated by the authors’ previous study [8], an adaptive and improved surrogate based optimization method using the ensemble of surrogates and HSR strategy (ISGO-HSR) is studied to enhance the efficiency and accuracy for solving the expensive black-box problems where the actual global optima are unknown beforehand. A new Latin hypercube type sampling method called TPSLE [9] is employed to generate the initial sample points to build the single and ensemble of surrogate models. Moreover, three various search subspaces: important local space (ILS), original global space (OGS) and promising joint space (PJS) are computed by HSR strategy. New points are supplemented to the sample set for sequentially improving the accuracy of prediction models. Tested using some representative benchmark optimization problems [10], ISGO-HSR method shows improved in identifying the global optimum.

2. ISGO-HSR method
An ensemble of surrogates based optimization approach using the HSR strategy is proposed to handle the complicated real-word engineering applications in the authors’ previous work [8]. The ensemble of surrogates can be obtained by dealing with the optimization formulation below

\[
\begin{align*}
\text{Find} & \quad \alpha, \beta \\
\min E_e & = \frac{1}{N} \sum_{k=1}^{N} \left( y(x_k) - \sum_{i=1}^{s} w_i \tilde{y}_i^{(k)}(x_k) \right)^2 \\
& = \frac{1}{s} \sum_{i=1}^{s} E_i, \\
E_i & = \frac{1}{N} \sum_{k=1}^{N} \left( y(x_k) - \tilde{y}_i^{(k)}(x_k) \right)^2, \\
\text{s.t.} & \quad E_i + \alpha \bar{E} > 0, \quad \alpha < 1, \quad \beta < 0
\end{align*}
\]

where \( E_i \) and \( E_e \) are the prediction sum of squares of root mean square (PRESSRMS) of the \( i \)th surrogate and the ensemble of surrogates separately, \( \bar{E} \) represents the average value of all surrogates’ PRESSRMS, \( N \) indicates the number of training points, \( x_k \) represents the \( k \)th sample point, \( y(x_k) \) and \( \tilde{y}_i(x_k) \) denote the true response and relevant prediction response from an ensemble of surrogates at the \( k \)th sample point respectively, \( \tilde{y}_i^{(k)}(x_k) \) indicates the approximated response of the \( i \)th single surrogate achieved by leave one out cross validation method. HSR strategy is conducted to identify the design subspaces OGS, PJS and ILS during each three iterations. In fact, the design subspaces PJS and ILS will speed up the convergence, and more promising points will be generated meat the actual optimal point. The detail description on OGS, PJS and ILS can be found in literatures [8].

It’s noted that the convergence criterion in this work is different from the authors’ previous paper [8]. In the authors’ previous paper, the actual global optima of all test examples are assumed to be known in advance. The convergence criterion is formulated as follows

\[
\begin{align*}
\begin{cases}
\left| \frac{f_{\text{opt}} - f_{\text{min}}}{f_{\text{min}}} \right| < \text{Tol}, & \text{if } f_{\text{min}} \neq 0 \\
f_{\text{opt}} < \text{Tol}, & \text{if } f_{\text{min}} = 0
\end{cases}
\end{align*}
\]

where \( f_{\text{min}} \) indicates the real global optimum, \( f_{\text{opt}} \) represents the current best solution, \( \text{Tol} \) is selected to judge whether the present best result satisfy the demand. The convergence criterion abovementioned is suitable for the real-world applications where the function characteristics are sufficiently gained. However, the global minima of most engineering design optimization problems like aerospace designs
are unknown beforehand. Therefore, the actual global optima of all test examples are supposed to be undiscovered in this study. The convergence criterion is changed as follows

\[ |\bar{F}_{i+1} - \bar{F}_{i}| \leq \varepsilon, \]

\[ \bar{F}_{i} = \frac{1}{5} \sum_{j=1}^{5} f_{j} \]

where \( f_{j} \) indicates the \( j \)th minimum prediction value, \( \varepsilon \) represents an allowable error determined by the researcher. If the improvement from the average of five minimum function values becomes negligible, the current best result is considered to be acceptable. This convergence criterion offers an efficient way to solve the expensive black-box problems.

The ISGO-HSR method improved from an existing ESGO-HSR approach is presented to well handle the most real-world applications without knowing the actual global optima. The global minima of all test examples are assumed to be undiscovered in this paper. More details of the ESGO-HSR approach can be found in the authors’ previous paper [8].

3. Results and discussions

The accuracy and efficiency of ISGO-HSR method are tested using six well-known benchmark optimization problems SC, GP, RB, HN6, TR10, F16 formulated below. All problems are considered as the expensive black-box problems whereas the actual global optima as well as the function characteristics are unknown in advance. All design parameters in ISGO-HSR method which can refer to the literature [8] are the same for all problems. Furthermore, \( \varepsilon \) is set to be 0.001 for all test problems.

1. Six-hump Camel-Back function (SC), \( n = 2 \)

\[ f(x) = 4x_{1}^{2} - 2.1x_{1}^{4} + \frac{x_{1}^{6}}{3} + x_{1}x_{2} - 4x_{2}^{2} + 4x_{2}^{4}, x \in [-2, 2], f_{\text{min}} = -1.0316 \]  

(4)

2. Goldstein and Price function (GP), \( n = 2 \)

\[ f(x) = \left[ 1 + (x_{1} + x_{2} + 1)^{2} \left( 19 - 14x_{1} + 3x_{1}^{2} - 14x_{2} + 6x_{1}x_{2} + 3x_{2}^{2} \right) \right]^{2} \]

\[ + 30 + (2x_{1} - 3x_{2})^{2} \left( 18 - 32x_{1} + 12x_{1}^{2} + 48x_{2} - 36x_{1}x_{2} + 27x_{2}^{2} \right), x \in [-2, 2], f_{\text{min}} = 3 \]  

(5)

3. Rosenbrock function (RB), \( n = 2 \)

\[ f(x) = 100 (x_{2} - x_{1}^{2})^{2} + (x_{1} - 1)^{2}, x \in [-2, 2], f_{\text{min}} = 0 \]  

(6)

4. Hartman function (HN6), \( n = 6 \)

\[ f(x) = \sum_{i=1}^{n} c_{i} \exp \left[ -\sum_{j=1}^{n} a_{ij} (x_{j} - p_{ij})^{2} \right], i = 1, 2, \ldots, n, x \in [0, 1], f_{\text{min}} = -3.3224 \]  

(7)

\[ \begin{bmatrix} a_{ij} \end{bmatrix} = \begin{bmatrix} 10 & 3 & 17 & 3.5 & 1.7 & 8 \\ 0.05 & 10 & 17 & 0.1 & 8 & 14 \\ 3 & 3.5 & 1.7 & 10 & 17 & 8 \\ 17 & 8 & 0.05 & 10 & 0.1 & 14 \end{bmatrix} \]

\[ \begin{bmatrix} p_{ij} \end{bmatrix} = \begin{bmatrix} 1312 & 1696 & 5569 & 124 & 8283 & 5886 \\ 2329 & 4135 & 8307 & 3736 & 1004 & 9991 \\ 2348 & 1451 & 3522 & 2883 & 3047 & 6650 \\ 4047 & 8828 & 8732 & 5743 & 1091 & 381 \end{bmatrix} * 10^{4} \]

5. Trid function (TR10), \( n = 10 \)

\[ f(x) = \sum_{i=1}^{n} (x_{i} - 1)^{2} - \sum_{i=2}^{n} x_{i}x_{i-1}, x \in [-100, 100], f_{\text{min}} = -210 \]  

(8)

6. A function of 16 variables (F16), \( n = 16 \)
\[ f(x) = \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{ij} \left( x_i^2 + x_j + 1 \right) \left( x_j^2 + x_i + 1 \right), \quad i = 1, \ldots, n, \quad x \in [-1, 1], \quad f_{\text{opt}} = 25.8750 \] (9)

The computational cost is generally direct proportion to the NFE for computation-intensive black-box problems. Thus, NFE is used for representing the search efficiency. Meanwhile, the optimal result \( f_{\text{opt}} \) obtained is also employed to indicate the optimization quality and accuracy. Ten runs are conducted for all test examples for eliminating the random variation. The optimal results are compared with two recently introduced SBGO approaches SEUMRE and HAM. The collected mean and scope values from the optimal results \( f_{\text{opt}} \) and NFE are recorded in Tables 1 and 2. The sign \( > \) means that at least one of the experiments fails to meet the convergence criteria expressed in Eq. (6) within 300 function evaluations. And, the values given in the parentheses indicate the amount of failures. The better mean values of \( f_{\text{opt}} \) and smaller NFE are highlighted with bold. Through analysing the test results in Tables 1 and 2, we can find that:

1. ISGO-HSR method can successfully achieve the acceptable optimal solutions for all test examples without knowing the actual global optima in advance.
2. ISGO-HSR method uses the least number of NFE for most problems. SEUMRE and HAM can only fast catch the global optima for simple problems as GP and RB. However, they require largest NFE for complicated problems including HN6, TR10 and F16, even fail to find the acceptable global optima.
3. ISGO-HSR method performs the superior capability for all test experiments. It’s more efficient and accurate than the comparative methods SEUMRE and HAM.

In ISGO-HSR method, the ensemble of surrogates is used to decrease the required evaluations of the expensive black-box functions. Meanwhile, the HSR strategy is used to accelerate the search in a smaller and more promising subspace. Therefore, the success rate of the optimization method ISGO-HSR is more superior than the comparative methods SEUMRE and HAM. The recently presented ISGO-HSR method shows satisfactory performance From the efficiency and accuracy perspectives.

4. Conclusions
An improved surrogate based optimization method ISGO-HSR has been presented to efficiently handle the expensive black-box problems in this study. The primary contributions are summarized as below:
1) Introduce an improved surrogate-based optimization method ISGO-HSR that can solve the expensive black-box problems where the function characteristics are unknown in advance.

2) The test results demonstrate that the proposed optimization method ISGO-HSR is efficient and superior in handling the expensive black-box problems.

### Table 1. Comparative results $f_{opt}$ obtained by all optimization methods

| Fun. | SEUMRE          | HAM          | ISGO-HSR      |
|------|-----------------|--------------|---------------|
| SC   | [1.0316, -1.0284] | -1.0309 [-1.0316, -1.0256] | -1.0309 [-1.0316, -1.0290] | **-1.0313** |
| GP   | [3.0000, 3.0104] | 3.0012 [3.0000, 3.0021] | **3.0003** [3.0000, 3.0020] | 3.0040 |
| RB   | [0.0000, 0.0395] | 0.0058 [0.0000, 0.0016] | 0.0003 [0.0000, 0.0007] | **0.0002** |
| HN6  | [-3.3221, -2.6475] | -3.1555 [-3.3223, -3.1622] | -3.2492 [-3.3223, -3.3191] | **-3.3216** |
| TR10 | [911.16, 2723.58] | 1883.87 [-209.19, -77.32] | -131.07 [-210.00, -210.00] | **-210.00** |
| F16  | [28.4079, 32.2758] | 30.4832 [25.9053, 26.7403] | 26.1413 [25.8758, 26.0356] | **25.9071** |

### Table 2. Comparative results NFE obtained by all optimization methods

| Fun. | SEUMRE          | HAM          | ISGO-HSR      |
|------|-----------------|--------------|---------------|
| SC   | [38, 69]        | 55.5         | 55.8          | 26, 66, **47.5** |
| GP   | [104, 146]      | 113.1        | 180.4         | 89, 168, **111.5** |
| RB   | [36, 118]       | 74.8         | 80.7          | 30, 105, **56.7** |
| HN6  | [36, 160]       | 118.9        | 156.7         | 70, 91, **77.5** |
| TR10 | (>300, >300)    | >300(10)     | >300(10)      | 162, 186, **171.7** |
| F16  | (>258, >300)    | >296.0(8)    | >300(10)      | 83, 110, **96.0** |

**Acknowledgments**

This research was supported by the National Science Foundation of China (Grant No. 61803306).

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