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Surrogate-based Design Optimization with Adaptive Sequential Sampling

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In spite of the recent developments in surrogate modeling techniques, the low fidelity of these models often limits their use in practical engineering design optimization. When surrogate models are used to represent the behavior of a complex system, it is challenging to simultaneously obtain high accuracy over the entire design space. When such surrogates are used for optimization, it becomes challenging to find the optimum/optima with certainty. Sequential sampling methods offer a powerful solution to this challenge by providing the surrogate with reasonable accuracy where and when needed. When surrogate-based design optimization (SBDO) is performed using sequential sampling, the typical SBDO process is repeated multiple times, where each time the surrogate is improved by addition of new sample points. This paper presents a new adaptive approach to add infill points during SBDO, called Adaptive Sequential Sampling (ASS). In this approach, both local exploitation and global exploration aspects are considered for updating the surrogate during optimization, where multiple iterations of the SBDO process is performed to increase the quality of the optimal solution. This approach adaptively improves the accuracy of the surrogate in the region of the current global optimum as well as in the regions of higher relative errors. Based on the initial sample points and the fitted surrogate, the ASS method adds infill points at each iteration in the locations of: (i) the current optimum found based on the fitted surrogate; and (ii) the points generated using cross-over between sample points that have relatively higher cross-validation errors. The Nelder and Mead Simplex method is adopted as the optimization algorithm. The effectiveness of the proposed method is illustrated using a series of standard numerical test problems.

Keywords: Cross-Over, Infill Criteria, Kriging, Sequential Sampling, Surrogate-based Design Optimization

I. Introduction

A. Surrogate-based Optimization

Design optimization problems often involve computationally intensive simulation models (high fidelity models) or expensive experiment-based system evaluations. Accurate surrogate models are effective tools for

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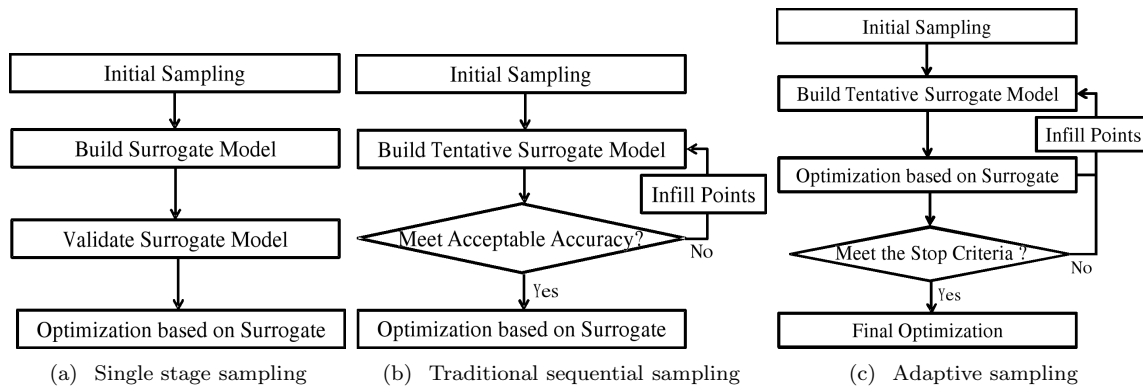


Figure 1. Surrogate-based optimization strategies

providing a tractable and an inexpensive approximation of the actual system evaluation. During the last two decades, the use of mathematical approximation models in design optimization has become popular for reducing the computational cost and filtering numerical noise of computationally intensive simulation models (high fidelity models).¹ This approximation model is known as a Surrogate or Metamodel (model of the models).² Popular surrogate modeling methods include Polynomial Response Surfaces,³ Kriging,^{4,5} Moving Least Square,^{6,7} radial basis functions,⁸ neural networks,⁹ and hybrid surrogate modeling.^{10,11} These methods have been applied to a wide range of disciplines, such as aerospace design, automotive design, chemistry, and material science.¹² The four main steps typically involved in constructing a surrogate model are: (a) choosing the appropriate method for performing the design of experiments (DoE); (b) evaluating the response of high fidelity simulation model at the sampling points; (c) determining the proper surrogate model to fit the responses in previous step; and (d) validating the accuracy of the surrogate model.

B. Design of Experiments

The fundamental issue in using a surrogate model in real-world engineering optimization is achieving sufficient accuracy across the entire design variable space. This accuracy, is often dependent on the DoE techniques used. There are many techniques to determine how to distribute the sample points, including Factorial and Central Composite designs,¹³ Latin Hypercube design,¹⁴ Orthogonal arrays,¹⁵ and Sobol sequence.¹⁶

There are three approaches for generating sample points in surrogate-based optimization,¹⁷ which are (i) Single stage sampling, (ii) Traditional sequential sampling, (iii) Adaptive sampling. These approaches are illustrated in Fig. 1. In the *Single stage* (or space filling) method, all the sample points are generated in one stage (Fig. 1(a)). This approach attempts to assign the locations of all sample points over the entire design space in one step. In the *Traditional sequential sampling* approach, sample points are generated in an iterative process (Fig. 1(b)). In this approach, a tentative (current) surrogate model is fitted to the response of a portion of the sample points and is updated at each iteration by including the response of new infill points (for improving the surrogate accuracy). In surrogate-based design optimization using single stage and traditional sequential sampling method, only one optimization process is involved. It is also important to note that the moving trust region concept used in traditional single stage method is not readily applicable to heuristic optimization where a population of solutions is used. In the *Adaptive sampling method* (Fig. 1(c)), the location information of the current global optimum at each iteration is also used for adding infill points and updating the surrogate model. In the literature, the word *sequential* is sometimes referred to as *adaptive* or *application driven*, and the new sample points are known as *infill points* or *update points*.

C. Sequential Sampling Review

In the case of SBDO using sequential sampling, the initial surrogate model is developed with a small number of sample points and is updated, in an iterative process, by adding new infill points. In this context, different criteria for determining the locations of the infill points are reviewed from the literature.^{18,19}

Currin et al.²⁰ proposed the Maximum Entropy sampling method. In this method, infill points are added to the initial sampling points in order to maximize entropy. Sacks et al.²¹ applied Mean Square Error

for finding the region with high errors to add infill points. This method, which is defined in a Gaussian based surrogate model like Kriging, can determine the location of the highest uncertainty of the surrogate model.²² Jones et al.²³ proposed an Expected Improvement(EI) function to generate infill points for a Kriging surrogate model. In this method, infill points are located where it has the maximum expected improvement value.

For surrogate-based design optimization, Jones et al.²³ proposed the Efficient Global Optimization (EGO) method based on the EI concept. In this method, which is also called sequential kriging optimization (SKO),²⁴ a Kriging surrogate model is fitted to the initial sampling points and infill points are added in the locations where the surrogate is minimized and the predicted error is relatively high. This most widely used approach is limited to Kriging, due to its ability for statistical interpretation that allows the measure of the possible error in the surrogate.

Among the sequential sampling methods that are not limited to a specific surrogate, Kleijnen et al.²⁵ used cross-validation error and Jackknifing variance²⁶ as the criteria. This method evaluates the variance between the surrogate and the high fidelity model and subsequently adds points in the area with the highest variance. Farhang-Mehr and Azarm²⁷ considered the region with a highly nonlinear response surface as a critical region to update sampling points. They determined this region as the location with higher variations in the surrogate. Rai²⁸ proposed the Qualitative and Quantitative Sequential Sampling technique in which the concept of a confidence function was used as the criterion for selecting infill points. In this case, the confidence function was a function of the designer's qualitative choices.

The trust-region approximation management framework (proposed by Alexandrov et al²⁹) and the surrogate management framework (proposed by Booker et al.³⁰) update the optimization solution by refining the surrogate at a predicted optimum using infill points. These methods focus the new sample points typically around the optimum region without paying significant attention to other regions of the design space.

D. Research Objective

Most of the existing sequential sampling approaches are designed for specific types of surrogate modeling techniques like Kriging. On the other hand, some sequential approaches add infill points only in the region of the current optimum. Such an approach often directs the optimization algorithm to an incorrect optimum region owing to sole dependency on the optimum region found in the early iterations. This issue is especially apparent in highly non-linear and multimodal problems.

The primary objective of this paper is to investigate a new methodology to perform surrogate-based design optimization using a sequential sampling method which is not limited to a specific kind of surrogate model. Hence, it can be applied to any kind of surrogate model including the hybrid models, such as Adaptive Hybrid Functions.¹¹ The proposed method adds infill points in the region of global optimum as well as in the location where the surrogate model has relatively high errors. The paper is organized as follows: Section II describes the formulation of the proposed methodology in detail. In this section, components of the overall methodology such as Kriging method, cross-validation, and cross-over techniques are briefly presented. In Section III, the proposed method is applied to a series of numerical test problems. The results are discussed in Section IV. Concluding remarks and future work are provided in Section V.

II. Adaptive Sequential Sampling Method

A. Methodology

The goal of the proposed approach in this paper is to develop an adaptive sampling method, which could enhance the effectiveness of surrogate-based optimization. According to this concept, there are two ways to enhance the accuracy of surrogate-based optimization: (i) adding infill points in the region where the optimum is located based on the low fidelity surrogate (local exploitation); and (ii) adding infill points over the whole domain of the design space to improve the global accuracy of the surrogate (global exploration).²² Key features of the Adaptive Sequential Sampling (ASS) method include:

1. The ASS method seeks to strike a balance between the two ways of adding infill points - i.e. balancing the exploitation and exploration.
2. Unlike most other sequential sampling methods which are developed based on Kriging method, the ASS method can be implemented in conjunction with different types of surrogate models.

The proposed methodology involves five major steps at each iteration, as described by the following steps.

Step 1: Sample the design space based on an *Investment Function* (IF). The IF is a criterion that defines the number and the location of infill points for the subsequent iterations. A set of initial sampling points are generated at the first iteration using design of experiment methods.

Step 2: Construct/Update the *Tentative Surrogate Model* (TSM). TSM is the surrogate model developed based on the current set of sample points in each iteration.

Step 3: Perform Global optimization based on the TSM. In this paper, the Nelder and Mead Simplex algorithm is adopted for this purpose.

Step 4: Check the stopping criteria. If the stopping criteria is satisfied, the current optimum is identified as the final optimum and the process is terminated. Otherwise, add infill points to the existing set of sample points, and go to step 5.

Step 5: Update the *Investment Function* value based on the optimum information and the accuracy of the TSM; and then repeat Steps 2, 3, and 4.

A flowchart of the algorithm is given in Fig. 2.

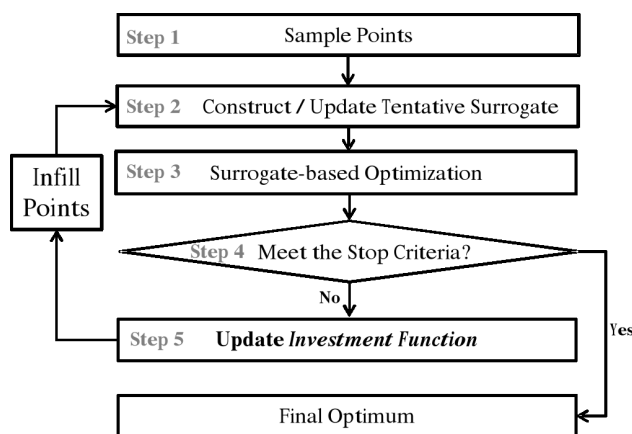


Figure 2. Adaptive sequential sampling method

B. Investment Function

This step is the most important and unique component of the ASS method. The *Investment Function* is the criterion for identifying the number and the locations of infill points in the design space. This function seeks to add infill points in the region: (i) around the global optimum of the tentative surrogate model; and (ii) between sample points with high levels of error to improve the global accuracy of surrogate model. After constructing the tentative surrogate model using the current set of sample points, an optimization algorithm and the cross-validation strategy are used to find the current global optimum and identify the points that have relatively higher levels of error, respectively. The *Investment Function* then adds infill points in the region of the the global optimum. It also adds infill points in the regions where the current surrogate has relatively lower fidelity.

C. Cross-Validation

Cross-validation (CV) errors are used to measure the global accuracy of the surrogate in the whole domain. According to the leave-one-out strategy,³¹ CV error for a specific sample point can be obtained by finding the difference between: (i) the actual response value at that point, and (ii) the response of the surrogate that is constructed by leaving out that point. The Related Accuracy Error (RAE) is used to evaluate the error at each training point. The RAE, for the sample point x_i , is given by

$$RAE(x_i) = \frac{|\tilde{f}(x_i) - f(x_i)|}{f(x_i)} \quad (1)$$

where $f(x_i)$ is the actual function value at x_i . In Eq. 1, $\tilde{f}(x_i)$ represents the response of the surrogate model when x_i is not used as a training point. In the ASS method, the RAE is used as the measure of error at the current sample points.

D. Cross-Over

The ASS method generates infill points using a cross-over operator that is adopted from evolutionary optimization algorithms (e.g. genetic algorithms). Cross-over is a technique used to produce new solutions from existing ones, such that certain (design) characteristics of the existing solutions are retained. In the ASS method, this operator is used to combine information from two current sample points with high levels of cross-validation error. Several cross-over operators have been reported in the literature. The Intermediate Recombination³² method is used in the ASS method. This technique is only applicable for real variables to combine the genetic material of two parents (points with high levels of CV error) and produce two offspring (infill points) randomly in the neighborhood of the parent points. In the Intermediate Recombination, the offspring is computed by:

$$Z_i = X_i\alpha_i + Y_i(1 - \alpha_i) \quad i \in (1, 2, \dots, N_{var}) \quad (2)$$

where the vectors X and Y are the parent sample points and Z is the offspring. The variable α represents a scaling factor, and is chosen randomly between the interval $[-d, 1 + d]$. In this study, the *standard* intermediate recombination is used and the value of d is assumed to be zero ($d = 0$). In the *standard* intermediate recombination method, the offsprings are likely located in the region spanned by the parents.

In this paper, after selection of the current points with high level of CV error, the process of cross-over is carried out between randomly selected nearest neighbors, among the set of points with high CV error. Since the cross-over operator results in two new points, the one that is farther away from the existing sample points is selected as an infill point.

E. Design of Experiments

In surrogate-based design optimization, the distribution of the sample points in design space has a considerable effect on the accuracy of the surrogate model and eventually the global optimum. In the ASS method, Latin Hypercube (LH) sampling³³ is applied to sample the whole design space in the first iteration (to generate the initial sample points). However, the ASS method can use other sampling methods that provide a well distributed coverage of the entire domain, such as: the Audzeand Eglais method³⁴ and the Sobols quasirandom sequence generator.³⁵

Latin hypercube sampling is a strategy for generating random sample points, which promotes a uniform representation of the entire variable domain.³³ A Latin hypercube sample contains n_p sample points (between 0 and 1) over m dimensions in a matrix of n_p rows and m columns. Each row corresponds to a sample point. The values of n_p points in each column are randomly selected - one from each of the intervals, $(0, 1/n_p), (1/n_p, 2/n_p), \dots, \text{and}(1 - 1/n_p, 1)$.³³

F. Surrogate Model

The proposed ASS method is not limited to a specific surrogate model. However, it is more readily applicable with interpolation methods, such as Kriging,³⁶ RBF,⁸ and E-RBF.³⁷ In this paper, the Kriging method is selected to implement the framework. Kriging is an interpolating method that is widely used for representing irregular data. The standard Kriging model is given by

$$\tilde{f}(x) = G(x) + Z(x) \quad (3)$$

where $\tilde{f}(x)$ is the approximation of the actual response $f(x)$; $G(x)$ is the known type of approximation function (often a polynomial); and $Z(x)$ is assumed to be a weak stationary stochastic process with zero mean and variance σ^2 .³⁸The $i, j - th$ element of the covariance matrix of $Z(x)$ is given as

$$COV[Z(x^i), Z(x^j)] = \sigma_z^2 R_{ij} \quad (4)$$

where R_{ij} is the correlation function between the i^{th} and the j^{th} data points; and σ_z^2 is the process variance. In the present paper, a Gaussian function is used as the correlation function, defined as

$$R(x^i, x^j) = R_{ij} = \exp \left\{ -\sum_{k=1}^{n_d} \theta_k \left(x_k^i - x_k^j \right)^2 \right\} \quad (5)$$

where the generic unknown parameter θ_k is distinct for each dimension, and is generally obtained by solving a nonlinear optimization problem.

G. Optimization Algorithm

The effectiveness of the ASS method is dependent on the global optimization algorithm which searches the optimum based on the current surrogate. In this paper, the Nelder and Mead Simplex algorithm³⁹ is applied for implementing the proposed methodology. This derivative-free and direct search method is used for minimizing unconstrained multivariable functions. It converges to an optimum by forming and using a simplex to search for promising directions. A simplex is defined as a geometrical figure formed by $N + 1$ vertices, where N is the number of function variables. In each iteration, simplex calculates a reflection point of the worse point through the centroid point. According to worst point value, the algorithm performs a reflection or extension, and a contraction or shrinkage to respectively form a new simplex and a new point to replace the worse point.⁴⁰

H. Surrogate-based Design Optimization using the ASS method

For the sake of simplicity, the following 1-D optimization problem²² is used to illustrate the implementation of the ASS method in SBDO.

$$f(x) = (6x_1 - 2)^2 \sin [2(6x_1 - 2)] \quad \text{where } x_1 \in [0 \ 1]$$

The function and its global optimum are shown in Fig. 3.

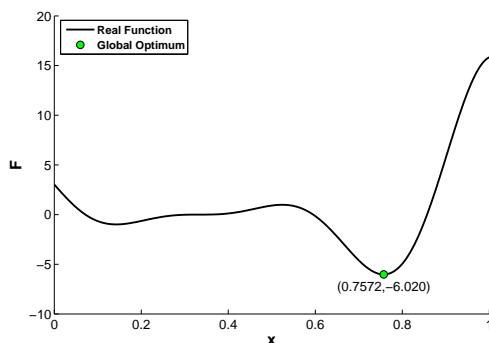


Figure 3. 1-D optimization problem

The following three different methods can be used as the stopping criteria: (i) the difference between optimum values of two consecutive iterations is smaller than a threshold value, (ii) the maximum number of sample points allowed (total investment) is reached, (iii) the change in the investment function value is smaller than a defined threshold value over consecutive iteration. In this paper, a predefined number of investment points (training points) is considered as the stopping criterion. The total number of sample points used to construct the surrogate for this function is assumed to be 9. The four main steps for constructing the surrogate based on the ASS method are as follows (illustrated in Fig. 4): (i) place 3 uniform points in the design space using the Latin Hypercube sampling method; (ii) construct the tentative surrogate and run optimization to find the current global optimum; (iii) add infill points in the region of the current optimum and in the region(s) with large cross-validation errors; and (iv) repeat steps (ii) and (iii) till the termination criterion is met (Fig. 4(d)). To investigate the reliability of the proposed ASS method for SBDO, a statistical study is carried out. In this study, 50 random sets of 9 Latin Hypercube sample (LHS) points are generated for the one-stage SBDO. The ASS method is carried out using 3 initial sample points and 6 infill points. The results are compared with Kriging using single stage sampling as summarized in Table 1.

Box plots are used to illustrate the performance of the SBDO. The statistical performance of both the ASS method and the single stage SBDO methods are shown in Fig. 5 (with 50 runs). In the box plots: (i) the central mark is the median, (ii) the edges represent the 25th and 75th percentiles, (iii) the ends of the vertical lines indicate the minimum and maximum data values, or 1.5 times of the inter-quartile in each

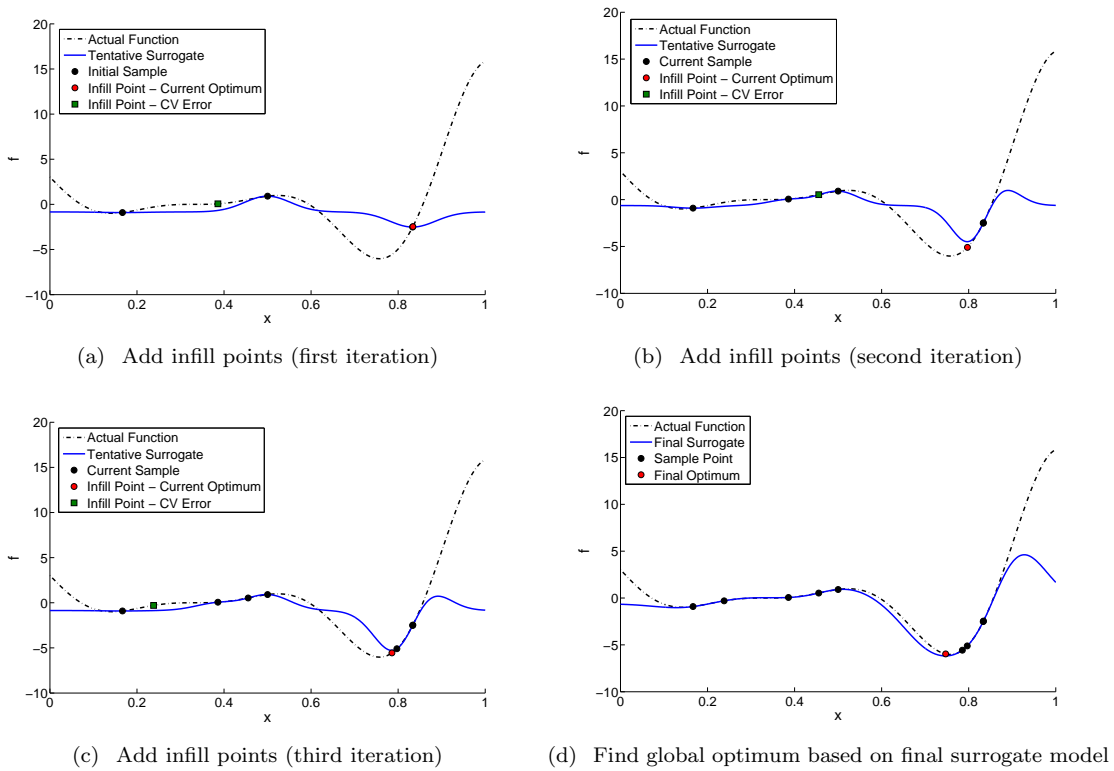


Figure 4. Implementation of the ASS method on 1-D optimization problem

Table 1. Comparison of the performances of ASS and single stage method on 1-D optimization problem (50 Trials)

Method Type	Optimum Design Variable		Objective Function	
	$AM(X)$	$\sigma^2(X)$	$AM(F)$	$\sigma^2(F)$
Single Stage	0.7185	0.0219	-5.5186	1.6261
ASS	0.7566	9.8618E-06	-6.0154	8.3208E-05
Analytical	0.7572		-6.0207	

AM =Arithmetic Mean, $\sigma^2()$ =Variance

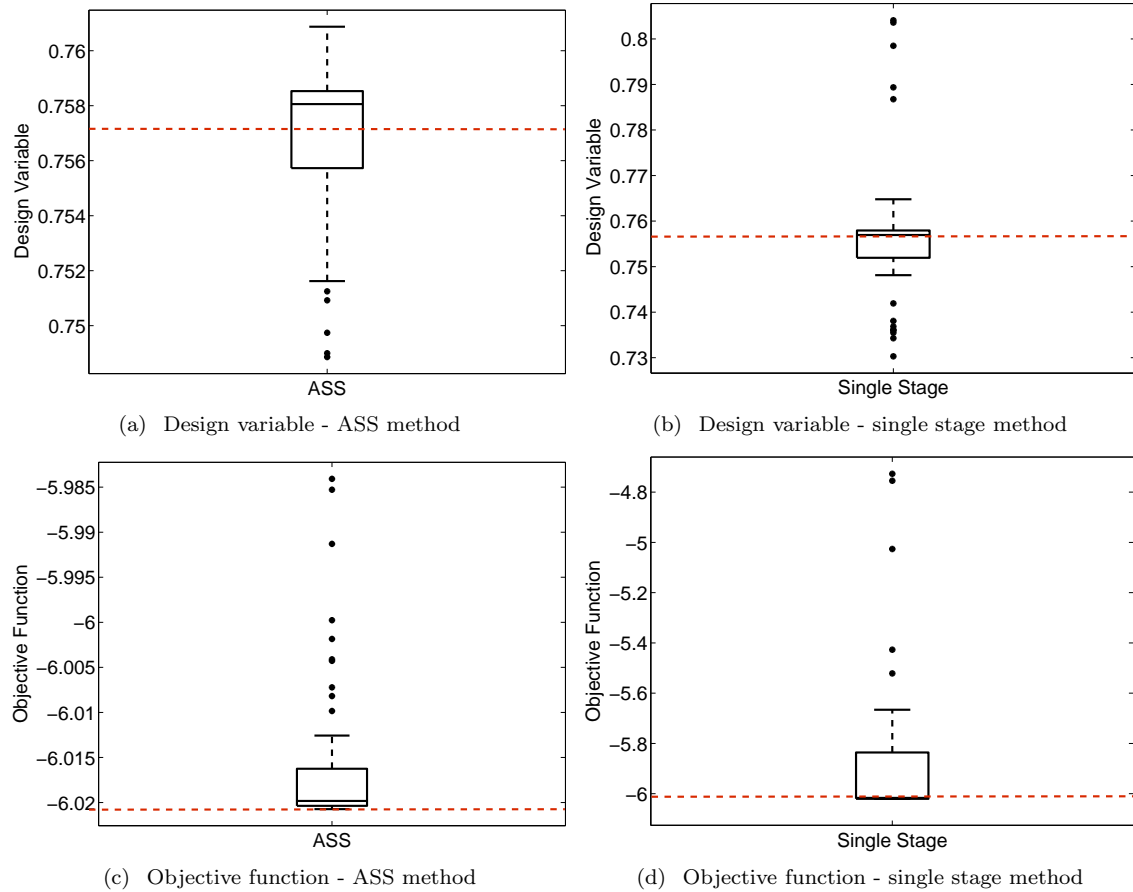


Figure 5. Box plots of objective function and design variable for ASS and single stage method

direction if the limit of the data falls beyond 1.5 times of the inter-quartile range, and (iv) the points outside the ends of the lines are outliers.

The box plot for design variables are shown in Figs. 5(a) and 5(b). The dashed red line represents the optimum design variable value. We observe that the variance of the design variable values (of 50 runs) using the ASS method is smaller than that using single stage method. Figures 5(c) and 5(d) show the objective function values. It can also be observed that the median value using the ASS method is closer to the actual optimum function value than that using the single stage method. Similarly in Table 1, according to the arithmetic mean of the results, the ASS method is also more accurate when compared to the single stage method. In addition, the deviation of the results over the 50 trials in the ASS-based Kriging is significantly less than that in the single stage-based kriging.

III. Numerical Examples

In this section, the proposed ASS method is validated using the following numerical test problems: (i) Booth function, (ii) Hartmann function with 3 variables,⁴¹ and (iii) Hartmann function with 6 variables.⁴¹ The expressions of these problems are summarized as follows.

Test Function 1: Booth Function

$$f(x) = (x_1 + 2x_2 - 7)^2 + (2x_1 + x_2 - 5)^2$$

where $x_1 \in [-10 \ 10]$, $x_2 \in [-10 \ 10]$

Test Function 2 and 3: Hartmann Function

$$f(x) = - \sum_{i=1}^4 c_i \exp \left\{ - \sum_{j=1}^n A_{ij} (x_j - P_{ij})^2 \right\} \quad (6)$$

$$\text{where } x = (x_1 \ x_2 \ \dots \ x_n) \quad x_i \in [0 \ 1]$$

The following cases are based on the number of design variables which include: (i) Hartmann-3 with 3 input variables (test function 2), and (ii) Hartmann-6 with 6 input variables (test function 3). When the number of variables, $n = 3$, c is given by $c = [1 \ 1.2 \ 3 \ 3.2]^T$, and A and P are given by

$$A = \begin{bmatrix} 3.0 & 10 & 30 \\ 0.1 & 10 & 35 \\ 3.0 & 10 & 30 \\ 0.1 & 10 & 35 \end{bmatrix}, \quad P = \begin{bmatrix} 0.3689 & 0.1170 & 0.2673 \\ 0.4699 & 0.4387 & 0.7470 \\ 0.1091 & 0.8732 & 0.5547 \\ 0.03815 & 0.5743 & 0.8828 \end{bmatrix} \quad (7)$$

When the number of variables, $n = 6$, c is given by $c = [1 \ 1.2 \ 3 \ 3.2]^T$, and A and P are given by

$$A = \begin{bmatrix} 10.0 & 3.0 & 17.0 & 3.5 & 1.7 & 8.0 \\ 0.05 & 10.0 & 17.0 & 0.1 & 8.0 & 14.0 \\ 3.0 & 3.5 & 1.7 & 10.0 & 17.0 & 8.0 \\ 17.0 & 8.0 & 0.05 & 10.0 & 0.1 & 14.0 \end{bmatrix} \quad (8)$$

$$P = \begin{bmatrix} 0.1312 & 0.1696 & 0.5569 & 0.0124 & 0.8283 & 0.5886 \\ 0.2329 & 0.4135 & 0.8307 & 0.3736 & 0.1004 & 0.9991 \\ 0.2348 & 0.1451 & 0.3522 & 0.2883 & 0.3047 & 0.6650 \\ 0.4047 & 0.8828 & 0.8732 & 0.5743 & 0.1091 & 0.0381 \end{bmatrix} \quad (9)$$

IV. Results and Discussion

In this section, the results of the single stage-based kriging method are compared with that of the ASS-based Kriging for all numerical examples. The numerical settings used to investigate the ASS-based Kriging method are given in Table 2. This table lists (i) the number of input variables, (ii) the initial investment (number of sample points), (iii) the number of iterations times the number of infill points at each iteration, and (iv) the predefined total investment.

In the 1D optimization problem illustrated in Section II, the ASS method starts the sequential process by investing 3 points as the initial sample points and adds 6 new points in 3 iterations (as mentioned in Sec.III. H). For the Booth Function and the Hartmann Function with 3 variables, the ASS method starts with 18 sample points. The process of sequential sampling adds 5 infill points at each iteration. The sequential process of adding infill points in the Booth Function is shown in Fig. 6. It is observed that: (i) the infill points cover the entire design space; (ii) all the infill points do not need to be close to the global optimum location. Finally, in the Hartmann Function with 6 variables, the ASS method uses 75 initial sample points and adds 75 infill points in 14 iterations. For each problem, box plots are used to show the variations of the results.

In the second numerical example (the Booth Function), the ASS method has similar results with the single stage method, as seen from Table 3. However, the variance in the ASS-based Kriging is less than that in the single stage-based Kriging, which is illustrated in Fig. 7. The maximum error in the objective function (among 50 runs) of the single stage kriging-based optimization is larger in the order of magnitude than that of the ASS-based optimization.

It is seen from Table 4 that when the ASS method is applied to the Hartmann Function with 3 variables, the accuracy of the obtained optimum is not significantly different with respect to the analytical results.

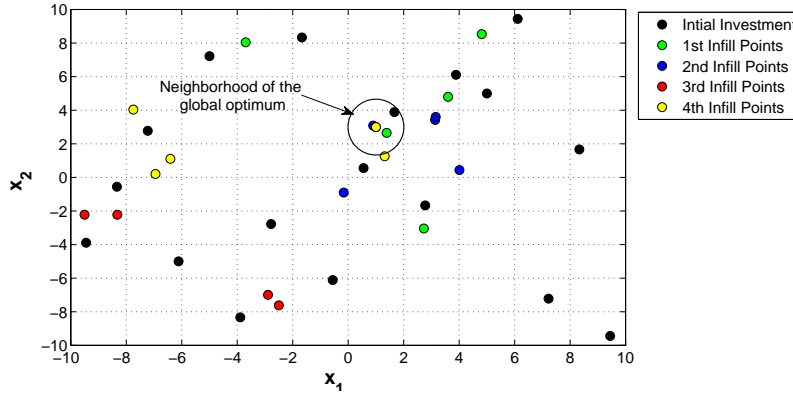


Figure 6. Infilling points based on ASS method in the Booth function

Table 2. Numerical setup for test problems

Function	No. of Variables	No. of Initial Investment	No. of Iteration \times Infill Points	Total No. of Investment
1-D Problem (No.1)	1	3	3×2	9
Booth Function (No.2)	2	18	4×5	38
Hartmann-3 Function (No.3)	3	18	4×5	38
Hartmann-6 Function (No.4)	6	75	5×14	150

Table 3. Comparison of the performances of ASS and single Stage method on Booth function by using Kriging surrogate model (50 Trials)

Method Type	Optimum Design Variables				Objective Function)	
	$AM(X_1)$	$\sigma^2(X_1)$	$AM(X_2)$	$\sigma^2(X_2)$	$AM(F)$	$\sigma^2(F)$
Single Stage	0.9997	6.903E-06	3.00	4.508E-06	2.5e-5	2.526E-09
ASS Method	0.9998	5.121E-07	3.00	1.952E-07	1.90e-6	1.981E-11
Analytical	1		3		0	

AM =Arithmetic Mean, $\sigma^2()$ =Variance

Table 4. Comparison of the performances of ASS and single stage method on Hartmann functions (3 Variables) by using Kriging surrogate model (50 Trials)

Method Type	Optimum Design Variables			Objective Function
	$AM(X_1)$	$AM(X_2)$	$AM(x_3)$	$AM(F)$
Single Stage	0.1929	0.5959	0.8303	-3.4586
ASS Method	0.3904	0.5909	0.8116	-3.6378
Analytical	0.1146	0.5556	0.8525	-3.8627

AM = Arithmetic Mean

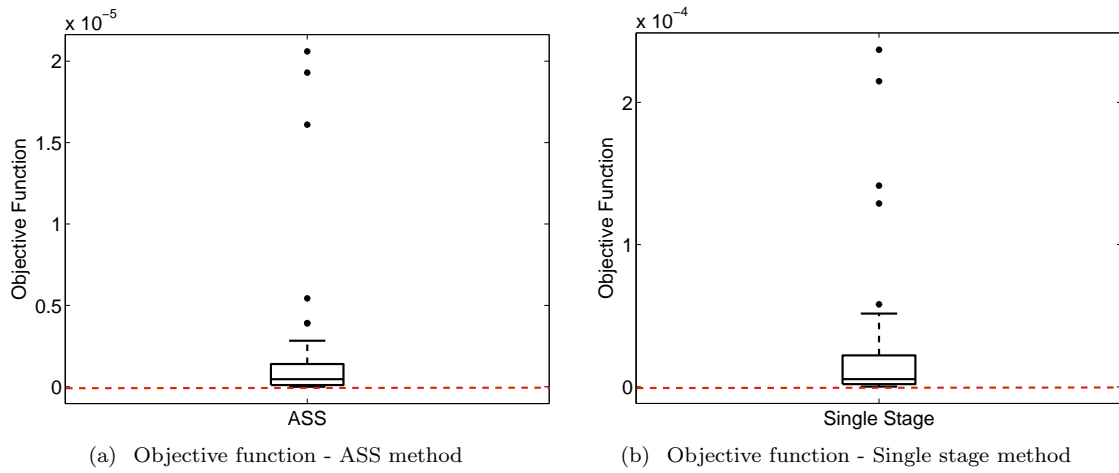


Figure 7. Box plots of objective function for ASS and single stage method of Booth function

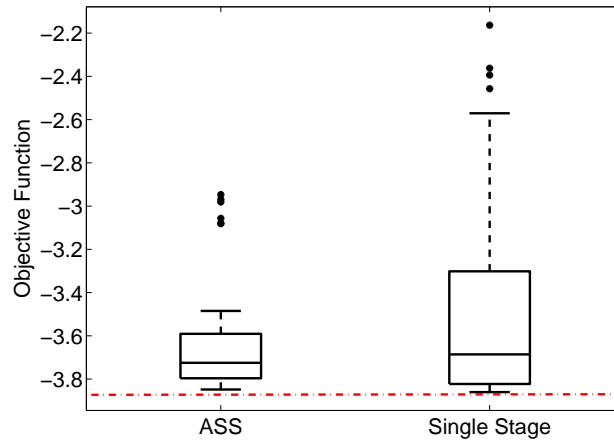


Figure 8. Box plots of objective function for ASS and single stage method of Hartmann Function with 3 Variables

However, the deviation of the optimization results over the 50 trials in the ASS-based Kriging is less than that in the single Stage-based kriging (as seen in Fig. 8).

Table 5 represents the results given by the ASS-based and the single stage-based Kriging for the Hartmann Function with 6 variables. The accuracy of the arithmetic mean of the optimum objective function value given by the ASS method is superior than that given by the Single stage-based method. Similarly, the deviation of the optimization results over the 50 trials in the ASS-based Kriging is also less than that in the single stage-based kriging (Fig. 9).

The percentage error of the results given by the ASS-based kriging for the numerical problems in the 50 trials are illustrated in Fig. 10. Expectedly, the error increases as the number of design variables increases. The Percentage Error(E_p) is given by

$$E_p = \left| \frac{F_{an} - F_{ASS}}{F_{an}} \right| \times 100 \quad (10)$$

where F_{an} represents the (analytically found) actual optimum objective value, and the F_{ASS} is the optimum objective value obtained by the SBDO using ASS.

Table 5. Comparison of the performances of ASS and single stage method on Hartmann functions (6 Variables) by using Kriging surrogate model (50 Trials)

Method Type	Optimum Design Variables						Objective Function
	$AM(X_1)$	$AM(X_2)$	$AM(X_3)$	$AM(X_4)$	$AM(X_5)$	$AM(X_6)$	$AM(F)$
Single Stage	0.3909	0.6440	0.6837	0.4555	0.3391	0.4355	-2.1459
ASS Method	0.3021	0.4995	0.4976	0.3883	0.3512	0.3915	-2.8637
Analytical	0.2016	0.1500	0.4768	0.2753	0.3116	0.6573	-3.3223

AM = Arithmetic Mean

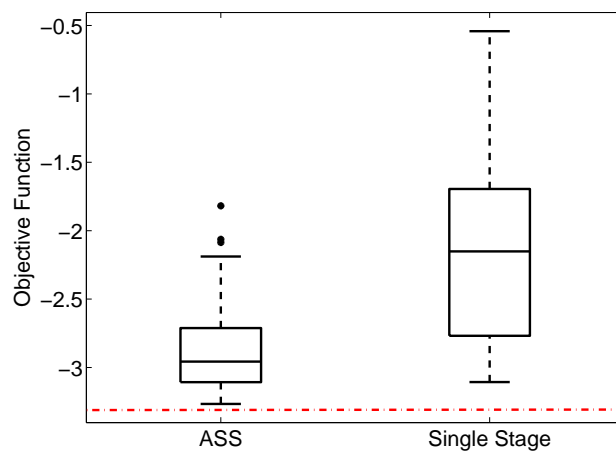


Figure 9. Box plots of objective function for ASS and single stage method of Hartmann function with 6 variables

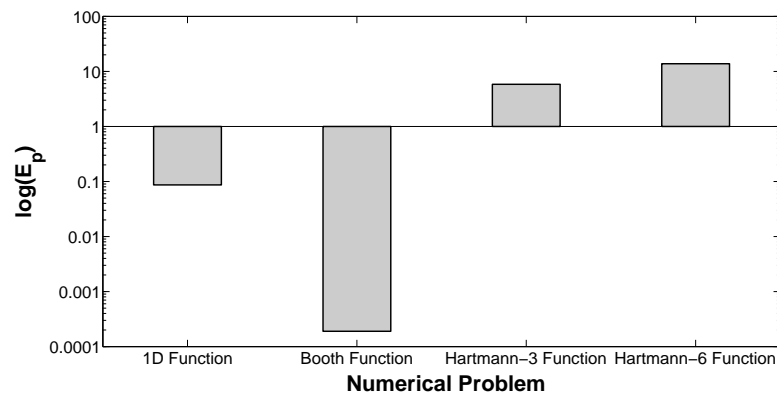


Figure 10. Percentage error between ASS-based Kriging and analytical result on numerical problems (50 Trials)

V. Conclusion

This paper presents an adaptive sampling method to efficiently and accurately find the optimum in surrogate-based design optimization, which we call the Adaptive Sequential Sampling (ASS) method. In this methodology, the local and the global accuracy of the surrogate model is improved by adding infill points. According to this framework, the initial tentative surrogate model is constructed over an initial set of uniform sample points. An *Investment Function*(*IF*) is defined as the criterion for determining the number and the location of infill points in each iteration. The IF depends on the cross-validation error of the current sample points in each iteration, and the location of the current global optimum. At each iteration, the IF adds one infill point at the optimum found in the previous iteration. In addition, the ASS method uses the cross-over operator to generate infill points between points with high cross-validation errors. In this paper, the global optimum is determined by implementing the Nelder and Mead Simplex algorithm. Cross-over is performed using intermediate recombination. A series of numerical problems are examined to validate and compare the performance of the ASS method with that of the single stage method. Preliminary results indicate that the ASS-based kriging method improves the efficiency and the accuracy of SBDO over the single stage method.

Future work may include applying other robust heuristic algorithms such as Particle Swarm Optimization to perform SBDO. The ASS method should be further extended to include special criteria for adaptively identifying the suitable number of iterations and the required number of infill points at each iteration during the SBDO process.

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