Research Article

Quality and Reliability Engineering International

(wileyonlinelibrary.com) DOI: 10.1002/qre.1432

Published online 25 June 2012 in Wiley Online Library

An Efficient Adaptive Sequential Methodology for Expensive Response Surface Optimization

Adel Alaeddini,[a*,†] Alper Murat,[b] Kai Yang[b] and Bruce Ankenman[c]

The preset response surface methodology (RSM) designs are commonly used in a wide range of process and design optimization applications. Although they offer ease of implementation and good performance, they are not sufficiently adaptive to reduce the required number of experiments and thus are not cost effective for applications with high cost of experimentation. We propose an efficient adaptive sequential methodology based on optimal design and experiments ranking for response surface optimization (O-ASRSM) for industrial experiments with high experimentation cost, limited experimental resources, and requiring high design optimization performance. The proposed approach combines the concepts from optimal design of experiments, nonlinear optimization, and RSM. By using the information gained from the previous experiments, O-ASRSM designs the subsequent experiment by simultaneously reducing the region of interest and by identifying factor combinations for new experiments. Given a given response target, O-ASRSM identifies the input factor combination in less number of experiments than the classical single-shot RSM designs. We conducted extensive simulated experiments involving quadratic and nonlinear response functions. The results show that the O-ASRSM method outperforms the popular central composite design, the Box–Behnken design, and the optimal designs and is competitive with other sequential response surface methods in the literature. Furthermore, results indicate that O-ASRSM's performance is robust with respect to the increasing number of factors. Copyright © 2012 John Wiley & Sons, Ltd.

Keywords: adaptive sequential experiment; response surface optimization; central composite design (CCD); Box–Behnken design (BBD); optimal design; min–max optimization; system of quadratic inequalities

1. Introduction

Response surface methodology (RSM), a popular experimental method, explores the relationships between a set of explanatory variables and one or more response variables. Although the method was first introduced by Box and Wilson,[1] its essential elements have remained unchanged in most applications. The RSM uses a sequence of designed experiments to obtain an optimal response. Given important factors, the RSM first locates a region of curvature (region of interest) using the steepest ascent method by fitting a linear model (often a fractional factorial design) at every iteration. In the second phase, once the region of interest is identified, RSM uses experiments from a second-order design (often a central composite design [CCD] built from a new factorial design) and fits a quadratic model to locate at least a local optimum where the response is improved.

Although CCD (as well as other typical RSM methods) offers ease of implementation and good performance over a wide range of applications, as the number of factors increases, the number of required design points increases dramatically. This limitation constitutes a major disadvantage in many applications, in particular, where the cost of experimentation is high or when the experimentation resources are limited (Gramacy and Lee,[2] and Gu[3]). For instance, in n dimensions, the full second-order model only has $(n^2+3n+2)/2$ terms,

$$y = \sum_{i=1}^{n} \beta_{ii} x_i^2 + \sum_{i,j=1}^{n} \beta_{ij} x_i x_j + \beta_0 \tag{1}$$

and the CCD requires $2^n + 2n + 1$ design points. The CCD is built by combining a factorial design with 2^n corner points, $2n$ star points on the axes and one center point (in some applications the center point is replicated to estimate measurement variability). Table I illustrates the number of terms in the quadratic model and the number of design points in CCD as the dimension increases.

To reduce the number of experiments needed, there have been some modifications and alternatives to the commonly used CCD design. For instance, Sanchez and Sanchez[4] proposed focusing only on the second-order terms, and Box and Behnken[5] proposed the

[a]*Industrial and Operations Engineering, University of Michigan, 1205 Beal Avenue, Ann Arbor, MI 48109, USA*
[b]*Industrial and Systems Engineering, Wayne State University, Detroit, MI, USA*
[c]*Industrial Engineering, Northwestern University, Evanston, IL, USA*
**Correspondence to: Adel Alaeddini, Industrial and Operations Engineering, University of Michigan, 1205 Beal Avenue, Ann Arbor, MI 48109, USA.*
[†]*E-mail: alaedini@umich.edu*

Table I. The increase in the number of terms in the quadratic model and number of design points in CCD as the dimension increases

No. dimensions	Terms in second-order model	Design points in CCD
3	10	15
4	15	25
5	21	43
6	28	77
7	36	143
8	45	273

more efficient Box–Behnken design (BBD). Although these methods are more efficient than CCD, they are not adaptive designs where new design points are selected sequentially and adaptively in a way that the optimum is determined by fitting the second-order model in a reduced region of curvature.

The main goal of this study is to develop an efficient experimentation method that locates the optimum point with as few observations as possible. This is achieved by modifying the second phase of RSM such that the select design points are selected adaptively and sequentially in the region of interest. The benefit of adaptive selection is to locate the optimum point in a local region of interest that is smaller than the original region and where a quadratic model provides a better approximation of the response. The proposed method is sequential, adaptive, and recursive, which first decomposes the original feasible region into hyper-rectangular subregions. Next, it tests and eliminates those subregions not containing the optimum. These subdivision and elimination steps are repeated until the remaining feasible subregion is sufficiently reduced and the optimum point can be accurately estimated by fitting a second-order model.

The rest of the article is organized as follows. In Section 2, we first briefly review the literature on advancements in RSM with special emphasis on the adaptive experimentation methods. In the later part of Section 2, we describe the optimal designs used as an integral component of the proposed methodology. In Section 3, we explain the proposed Optimal Design-Adaptive Sequential Response Surface Methodology (O-ASRSM) methodology and its two core components (nonparametric and parametric strategy) in detail. In Section 4, we present the results of applying the O-ASRSM method to the simulated experiments and compare with those of the A-, D-, and V-optimal designs, classical BBD and CCD, and selected sequential design approaches from the literature. Finally, in Section 5, we discuss results and present future research directions.

2. Related literature

In this section, we briefly review the literature for adaptive sequential methodology for response optimization with a focus on data-efficient methods. In this regard, we first review classical response surface methods. Next, we discus more advanced adaptive and sequential methods. Finally, we present optimal designs as one of the components of the proposed approach.

2.1. *Classical RSM: CCD and BBD*

As a very effective tool for process optimization, RSM was introduced by Box and Wilson.[1] Because the literature on RSM is vast, the interested reader may be referred to good review studies in the literature. Myers *et al*.[6] and Myers[7] discuss the RSM advancements from the early 1970s to the late 1990s. Myers *et al*.[8] also presents a retrospective and literature survey on RSM.

According to Box and Behnken,[5] CCD is the most popular class of designs. As discussed earlier, the CCD consists of a 2^k factorial or fractional factorials of resolution V with n_F runs, $2k$ axial or star runs, and n_C center points, where k is the number of variables. The CCD requires two parameters that are the distance a of the axial runs from the design center and the number of center points. Usually the distance a is set as $(n_F)^{1/4}$ to make the design rotatable and three to five runs are recommended.[9]

As noted previously, one problem with CCD is the number of required experiments required for fitting the second-order model, especially when the number of variables increases. To increase the efficiency, there is a class of methods incorporating a fraction of CCD points, known as small composite designs. However, the small composite design has significant difficulty in estimating linear and interaction coefficients.[10] Another alternative for CCD is the BBD, which requires the number of variables to be greater than two[5] and combines 2^k factorials with incomplete block designs. However, there are no points at the vertices of the region where each variable attains upper and lower limits.

2.2. *Adaptive and sequential RSM*

The general philosophy of sequential design and learning through a retrospective study of RSM origin is discussed by Box.[11] The first sequential experimentation approach is presented by Box and Wilson,[1] where the experimental points are sequentially moved along the gradient direction based on a two-level factorial or fractional factorial design, followed by an addition of axial points when the lack-of-fit test indicates curvature in the system. The evolutionary operation, another adaptive experimental approach proposed in Box[12] and Box and Draper,[13] iteratively builds a response surface around the optimum from the previous iteration by drifting factorial experiments with center points. Both these approaches are primarily used for shifting the region of interest close to the optimum and replicate the same experimental design iteratively in different regions of the factor space (FS). Spendley *et al*.[14] proposed a simplex design instead of a factorial pattern as by Box[12] in optimization and evolutionary operation.

Friedman and Savage[15] proposed the one-factor-at-a-time (OFAT) approach, which changes one variable at a time while keeping others constant at fixed values to find the best response. In this method, once a factor is changed, its value is fixed in the remainder of the process, for example, no recurring changes. This process is repeated until all the variables are changed. However, OFAT experimentation is generally discouraged in the literature in comparison with factorial design and fractional factorial design (Box *et al*.,[16] Montgomery,[9] and Czitrom[17]). Frey *et al*.[18] introduced the adaptive OFAT (AOFAT) experimentation method, which tends to achieve greater gains than those of orthogonal arrays when experimental error is small or the interactions among control factors are large. Frey and Jugulum[19] investigate the mechanisms by which AOFAT technique leads to improvement. They investigated conditional main effect, exploitation of an effect, synergistic interaction, antisynergistic interaction, and overwhelming effect. The AOFAT method is shown to exploit main effects if interactions are small and exploits two-factor interactions when two-factor interactions are large (Frey and Wang[20]).

Another adaptive experimentation method is the adaptive response surface method, where in each iteration a portion of the design space that corresponds to the response values worse than a given threshold value is discarded.[21] When the underlying function is quasi-convex, such elimination reduces the design space gradually to the neighborhood of the global design optimum. However, the number of required design experiments increases exponentially with the number of design variables because adaptive response surface method uses CCD at each iteration and does not inherit any of the previous runs and requires a completely new set of CCD points. Wang[22] substitutes CCD with Latin hypercube design to keep some of the points from earlier runs and increase the efficacy. The successive RSM method uses a subspace of the original design as the region of interest to determine an initial approximate optimum, which is then improved during the subsequent stages.[23] In this method, the new region of interest is centrally built around each successive optimum. The improvement in response is attained by moving the center of the region of interest as well as changing its size through panning and zooming operations, respectively. At each subregion, a D-optimal experimental design is used to best use the number of available runs together with oversampling to maximize the predictive capability.

To reduce the number of experiments and avoid strong assumptions on the form of the response function, Moore *et al*.[24] designed a response optimization algorithm. Their algorithm tries to determine convex region of interest for performing experiments in each iteration. To define a neighborhood, they used a geometric procedure that captures the size and shape of the zone of possible optimum location(s). Anderson *et al*.[25] developed an efficient nonparametric approach called pairwise bisection for optimizing expensive noisy function. Their algorithm uses a nonparametric approach to find a geometric relationship among experimented points to find the optimum effectively. Alaeddini *et al*.[26] proposed an adaptive sequential methodology for responses with two factors, which combines the concept of bisection method and classical response surface optimization for reducing the number of required experiments for estimating the optimal point. Their methodology uses the information from previous experiments to shrink the FS toward the real optimum and identify the factor settings of new experiments.

Another adaptive and sequential experimentation research stream that emerges from computer experiments are called *surrogates* and extensively used in multidisciplinary design optimization. Sobieszczanski-Sobieski[27] proposed concurrent subspace optimizations, where the multidisciplinary systems are linearly decoupled for concurrent optimization. Renaud and Gabriele[28] modified this algorithm to build response surface approximations of the objective function and the constraints. Rodríguez *et al*.[29] introduced a general framework for surrogate optimization with a trust-region approach. Jones *et al*.[30] proposed an efficient global optimization of expensive black box functions. Alexandrov *et al*.[31] developed a trust-region framework for managing the use of approximation models in optimization. Chang *et al*.[32] suggested a stochastic trust-region response-surface method. Gano and Renaud[33] introduced a kriging-based scaling function to better approximate the high fidelity response on a more global level. Rodríguez *et al*.[34] suggested two sampling strategies, for example, variable and medium fidelity samplings for global optimization. Baumert and Smith[35] used pure random search for the global optimization of noisy functions and to assess the implications to stochastic global optimization. Jones[36] presented a taxonomy of existing approaches for using response surfaces for global optimization. We refer the reader to Sobieszczanski-Sobieski and Haftka,[37] Kleijnen,[38] Kleijnen *et al*.,[39] Simpson *et al*.,[40] and Chen *et al*.[41] for additional reviews of the studies in this field.

2.3. *Optimal design and space-filling sampling*

There are multiple optimal designs that differ by the statistical criterion used to select the experiment points. The points are selected by first determining the region of interest, selecting the number of runs to make, specifying the optimality criterion, and choosing the design points from a set of candidate points spaced over the feasible design region. The two earlier studies that greatly contributed to the development of the idea of optimal designs are Kiefer[42,43] and Kiefer and Wolfowitz.[44] Optimal designs offer three advantages over suboptimal experimental designs[45]: (i) optimal designs reduce the costs of experimentation by allowing statistical models to be estimated with fewer experimental runs; (ii) optimal designs can accommodate multiple types of factors, such as process, mixture, and discrete factors; and (iii) optimal designs can be optimized with constrained design space, for example, when the mathematical process space contains factor settings that are practically infeasible.

It is known that the least squares estimator minimizes the variance of mean-unbiased estimators. In the estimation theory for statistical models with one real parameter, the reciprocal of the variance of an (efficient) estimator is called the Fisher information for that estimator. Because of this reciprocity, minimizing the variance corresponds to maximizing the information. When the statistical model has several parameters, however, the mean of the parameter estimator is a vector, and its variance is a matrix. The inverse matrix of the variance matrix is called the information matrix. Because the variance of the estimator of a parameter vector is a matrix, the problem of minimizing the variance is complicated. Using statistical theory, statisticians compress the information matrix using real-valued summary statistics; being real-valued functions, these information criteria can be maximized. The traditional optimality criteria are invariants of the information matrix; algebraically, the traditional optimality criteria are functions of the eigenvalues of the information matrix.[46]

D-optimal design is the most widely used criterion in optimal designs. A design is said to be D-optimal if $|(X'X)^{-1}|$ is minimized, which is equivalent to minimizing the volume of the joint confidence region of the vector of regression coefficients or equivalently maximizing the differential Shannon information content of the parameter estimates.[47] A-optimality seeks to minimize the trace of the inverse of the information matrix (Min $tr(X'X)^{-1}$). This criterion results in minimizing the average variance of the estimates of the regression coefficients. Two other optimal criteria are the G-optimal design that minimizes the maximum scaled prediction variance over the design region and the *V*-optimal design that minimizes the average prediction variance over the set of points of interest. More recently, Ginsburg and Ben-Gal[48] suggest a new design-of-experiment optimality criterion, termed Vs-optimal, for the robust design of empirically fitted models. Pukelsheim[46] provides an excellent source on the optimal design of experiments.

Space-filling designs attempt to spread out the samples as evenly as possible to collect as much information about the entire design space as possible. Space-filling methods include orthogonal arrays and various Latin hypercube designs. Latin hypercube is a statistical method for generating a distribution of plausible collections of parameter values from a multidimensional distribution.[49] The technique was introduced by McKay *et al*.[50] and further developed by Iman *et al*.[51] More information on the Latin hypercube can be found in the studies of Tang,[52] Park,[53] and Ye *et al*.[49] In the context of statistical sampling, a square grid containing sample positions is a Latin square if and only if there is only one sample in each row and each column. A Latin hypercube is the generalization of this concept to an arbitrary number of dimensions, whereby each sample is the only one in each axis-aligned hyperplane containing it. Orthogonal sampling adds the requirement that the entire sample space must be sampled evenly.[54,55] In other words, orthogonal sampling ensures that the ensemble of random numbers is a very good representative of the real variability. Although orthogonal sampling is generally more efficient, it is more difficult to implement because all random samples must be generated simultaneously.

3. Proposed methodology

O-ASRSM starts with few experiments generated based on an optimal design followed by a nonparametric experiment ranking strategy and a parametric quadratic model fitting strategy. The purpose of ranking the experiments is to eliminate those parts of the FS that are unlikely to contain the real optimal point. The fitting of the quadratic model, which is concurrent to the experiment ranking, finds the approximate location of optimal point. The information from these strategies is combined to determine a reduced FS for the next run. This procedure continues until the convergence criteria based on the estimated optimal experiment are attained. In the rest of this section, we first describe the terminology and state the assumptions in Section 3.1. Next, we provide an overview of the methodology in Section 3.2 and then describe the two core strategies of the O-ASRSM: (i) nonparametric approach in Sections 3.3.–3.6 and (ii) parametric approach in Section 3.7. In Section 3.8, we describe how the results of these two strategies are used in designing the next run of O-ASRSM.

3.1. *Terminology and assumptions*

For ease of exposition, we first present the definitions and the terminology used in the proposed O-ASRSM method in the next section. Figure 1 illustrates some of the notations for a two-dimensional FS with five initial experiments:

r : index of runs, for example, $r = 1, 2, \ldots R$, where R is the total number of runs.
FS_r : factor space at run r and expressed as Cartesian product of factor ranges in run r.
n : number of factors in the FS.
fs_i : initial range of factor i.
D : design of the incumbent run.
d : minimum number of required points to estimate quadratic regression parameters ($d = (n^2 + 3n + 4)/2$).
e : index of experiments, for example, $e = 1,2,\ldots,E$, where E is the total number of experiments.
B : experiment with the best response level in a given run.

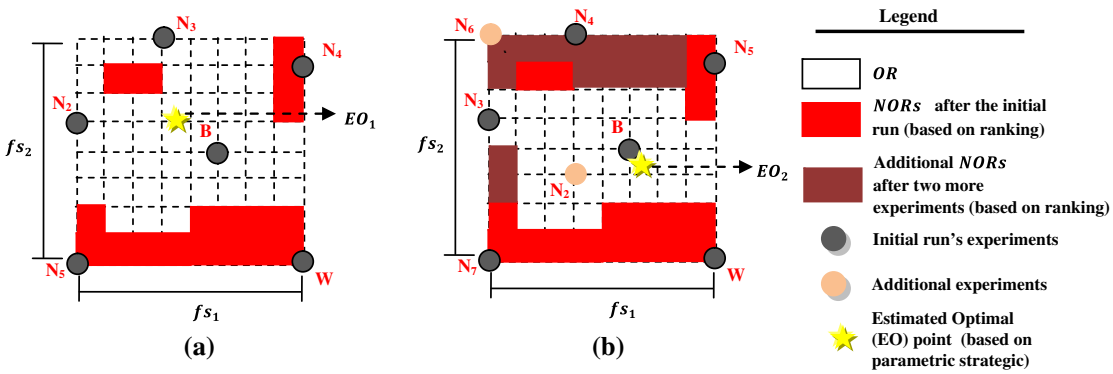


Figure 1. An illustration of terminology on a two-dimensional FS: (a) eliminated subregions (NORs) after first five experiments; (b) eliminated subregions (NORs) after additional two experiments

N_k : experiment with the kth best response level ($2 \leqslant k \leqslant e-1$) in a given run.
W : experiment with the worst response level in a given run.
OR_r : optimal region after the rth run.
NOR : nonoptimal region, for example, regions declared as not containing the optimum experiment.
RO : real optimum experiment of the response function.
EO_r : estimated optimum experiment at the end of the rth run.
sb : index of subregions for a given factor, for example, $sb = 1, 2 \ldots, k^n$, where k^n is the total number of subregions
E^* : total number of augmenting experiments.
S_{sb} : size of subregion sb.

The proposed O-ASRSM method, as in most RSM approaches, relies on the simplifying assumption of quadratic relation between the single response and the input factors. The reason is that RSM models are usually used in a sufficiently small region around the optimum experiment. As a result, it is commonly assumed in RSM applications that the underlying model can be approximated via a quadratic function in the small region of interest containing the optimum experiment. Such assumption also holds for this study; however, as shown in the numerical example section, the proposed method is robust with regard to this assumption.

3.2. *General scheme of the proposed methodology*

We illustrate the general scheme of the proposed methodology in Figure 2. The procedure is initialized with a region of interest, for example, an FS assumed to contain the optimum. The goal is to arrive at the vicinity of RO in finite number of experiments. The initial run is setup with an optimal design (D) using minimum number of experiments possible and then augmented with E^* additional experiments. Once the experimentation is completed, the approach follows two concurrent (parallel) strategies: (i) nonparametric ranking strategy and (ii) parametric model fitting strategy.

The main objective of the nonparametric strategy is to identify those parts of the FS that have a small probability of containing the real optimal point. For this purpose, the nonparametric strategy partitions the FS into a set of subregions (sb). Next, it uses the observed rank of experiments to construct a system of quadratic inequalities for each sb to check their possibility of containing the real optimal point (RO). In Section 3.4, we prove that the feasible solution of the system of equation for each sb is equivalent to the sb containing the RO and *vice versa*. The subregions that do not contain RO are indicated as NORs and the rest are labeled as ORs. Therefore, by applying the nonparametric strategy, the NORs are excluded from further experimentation in the subsequent iterations.

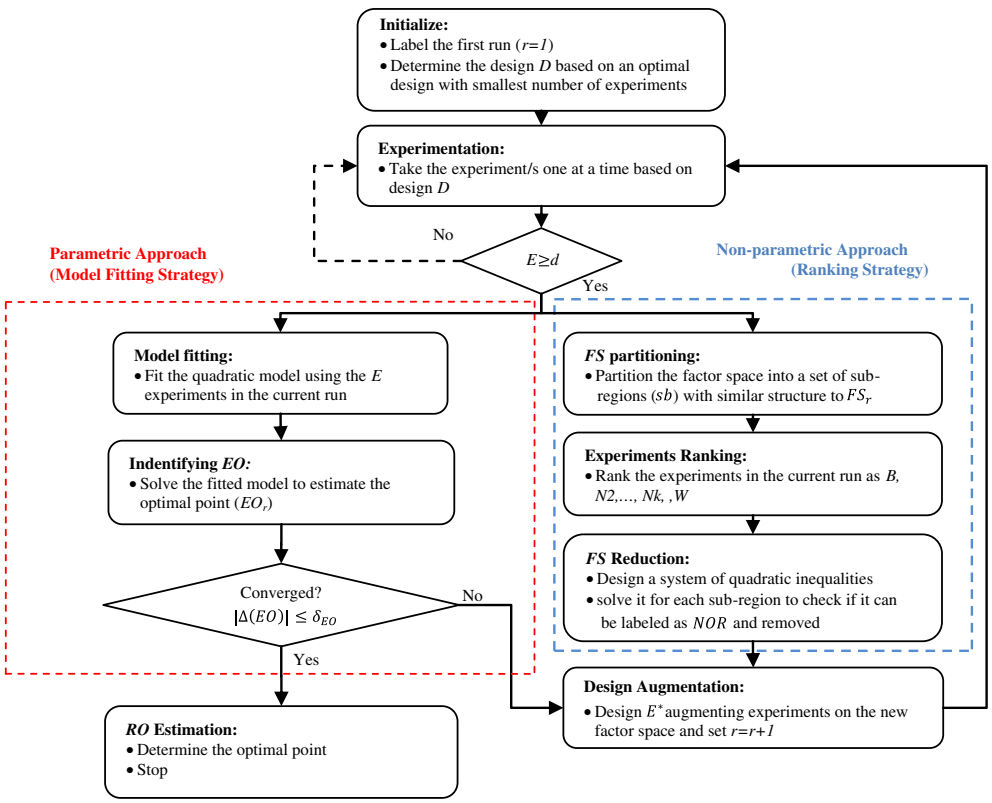


Figure 2. The general scheme of O-ASRSM

The main objectives of the parametric strategy are providing a point estimate (EO) of the real optima and checking the convergence of the algorithm. The parametric strategy fits a quadratic model using all the experiments and determines the EO. Next, it checks the convergence of the algorithm based on the incremental change in the ($|\Delta(EO)| \leqslant \delta_{EO}$).

On the basis of the result of parametric strategy, if the stopping a criterion is not met ($|\Delta(EO)| \leqslant \delta_{EO}$), the O-ASRSM algorithm proceeds to another run of experimentation and analysis by determining a reduced FS (FS_{r+1}) for of the next run ($r+1$) using only the ORs indentified by the nonparametric strategy. This procedure continues until the convergence criteria, incremental change in the *EO* being less than the tolerance specified, is attained.

3.3. *Design structure of experimental runs*

The design *D* structure of the FS in the proposed approach is adapted from the D-optimal design using minimum number of experiments. This design may be further augmented with E^* additional experiments in the identified *ORs* of the FS as discussed in Section 3.7.

The FS of each run *r* (FS_r) can be expressed as a mapping (φ_r) of the FS of the preceding iteration (FS_{r-1}). In its most general form, the proposed methodology generates a nested series of FSs, for example, $FS_r = \varphi_r(\varphi_{r-1}(\ldots\varphi_0(FS_1)))$. The output of mapping φ_r? depends on the current FS, the experimentation design (*D*), the experiment ranking outcome, and the result of the parametric strategy described in the next section. The ranking and the parametric strategies are described in Sections 3.4 and 3.8, respectively.

In the traditional CCD and BBD approaches, the corner points are taken at ± 1 unit distance away from the center point (0,0). In contrast, the proposed methodology, whenever it is possible, starts with a broader initial region around the center point, for example, $\pm 2^{n/4}$ unit distance from the center. The preceding relation is based on the calculation of axial points in rotatable CCD with single replicate at all designated points.[9] While initializing with a larger space may appear to be disadvantageous for O-ASRSM, our experimental results demonstrate that the reduction in the FS with the equal number of experiments well compensates for this difference. As an additional benefit, this modification may decrease the effect of random error on the initial results. To illustrate this, let us consider the diagonal cross section of these two designs in one dimension and assume that the noise is identically distributed on this cross section (Figure 3b). Then, it can be shown that the impact of the noise in predicting the optimal experiment point is less with the O-ASRSM's expanded FS. Figure 3 compares the initial FS of the traditional CCD and the proposed approach for a two-dimensional FS.

3.4. *Nonparametric approach: ranking strategy*

At each stage of the O-ASRSM, we rank the experiments according to their response levels, for example, from best (B) to worst (W), and the rankings in between are labeled as $N2\ldots, N(k-1)$. On the basis of this ranking, we remove the nonpromising subregions (NORs) from further consideration as they are determined to not to contain the RO. The remaining subregions identify an implied optimal region that contains the EO_r. This region, which is contained in FS (can be a convex or nonconvex set), determines the FS of the next run. In what follows, we first present the theorem used for the identification of the NORs inside an FS. Next, we describe how to reduce the FS by removing the nonoptimal subregions. Finally, we describe how to choose additional experiments in the final step of the nonparametric ranking strategy.

Theorem 1:

Let FS be a hyper-rectangular region of n dimensions with E experiments placed inside the region based on an optimal design. Also, assume E is greater than or equal to the minimum number of the required points to estimate quadratic regression parameters $E \geqslant d$. If the underlying function is quadratic and convex, and the true ranking of experiments is available, then using the ranking at least one subregion of nonzero size $\{S_{sb} | S_{sb} > 0, sb \in \text{FS}\}$ can be identified inside *FS* which is guaranteed not to contain the RO.

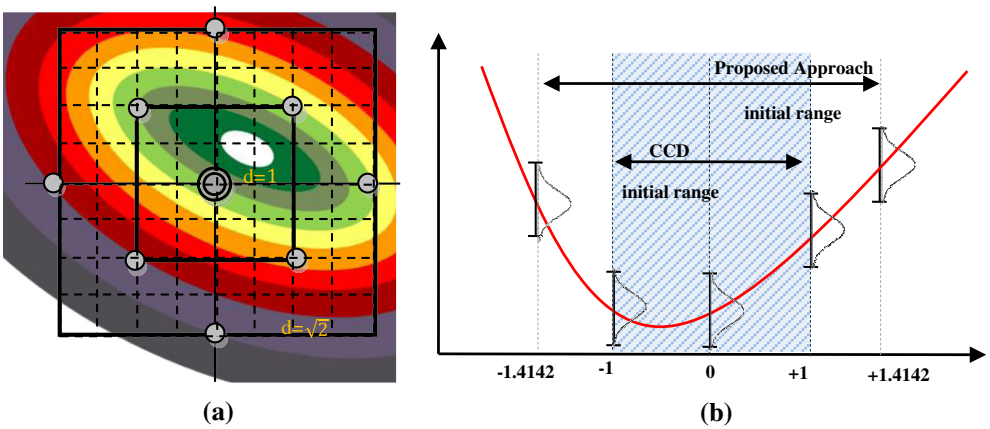


Figure 3. (a) Initial FS and design structure and (b) diagonal cross section of the traditional CCD and proposed O-ASRSM approach

Proof

Divide the hyper-rectangular FS into a set of k^n ($k > 1$) subregions with equal sizes ($dx_{1,\ldots,}\ dx_n$) in all dimensions. Because the underlying function is assumed to be convex and unimodal, there is only one subregion containing the RO, and $k^n - 1$ subregions not containing RO. It should be noted that because we use optimal design for *D*, the experiments are expected to not form a cluster in any subregion of the FS. If not, we can resize those subregions such that each experiment is contained in only one subregion.

Let us assume the optimal point, denoted by $\hat{O}$, resides in the subregion containing *W*, the worst experiments. Then, for each experiment $1 < e \leqslant E$, we express the response model in a canonical form as $Z_e = \sum_{i,j=1}^{n} A_{i,j}\left(X_i^e - X_i^{\hat{O}}\right)\left(X_j^e - X_j^{\hat{O}}\right) + \sum_{i=1}^{n} B_i\left(X_i^e - X_i^{\hat{O}}\right) + R^e$, where $A_{i,j} \in R$ and R^e are constants. Because the canonical form must be consistent with empirical ranks of the experiments $(B < N_2 < \cdots < N_k < W)$, we can sort the canonical forms of the experiments in an ascending order $\left(Z_{e_B} < Z_{e_{N_2}} < \cdots < Z_{e_W}\right)$. Next, on the basis of the sorted experiments, we formulate a system of inequalities with $E(E-1)/2$ pairwise comparisons as follows:

$$\begin{cases} Z_{e_B} - Z_{e_{N_2}} = \left[\sum_{i,j=1}^{n} A_{i,j}\left(X_i^{e_B} - X_i^{\hat{O}}\right)\left(X_j^{e_B} - X_j^{\hat{O}}\right) + \sum_{i=1}^{n} B_i\left(X_i^{e_B} - X_i^{\hat{O}}\right)\right] - \left[\sum_{i,j=1}^{n} A_{i,j}\left(X_i^{e_{N_2}} - X_i^{\hat{O}}\right)\left(X_j^{e_{N_2}} - X_j^{\hat{O}}\right) + \sum_{i=1}^{n} B_i\left(X_i^{e_{N_2}} - X_i^{\hat{O}}\right)\right] < 0. \\ Z_{e_{N_2}} - Z_{e_{N_3}} = \left[\sum_{i,j=1}^{n} A_{i,j}\left(X_i^{e_{N_2}} - X_i^{\hat{O}}\right)\left(X_j^{e_{N_2}} - X_j^{\hat{O}}\right) + \sum_{i=1}^{n} B_i\left(X_i^{e_{N_2}} - X_i^{\hat{O}}\right)\right] - \left[\sum_{i,j=1}^{n} A_{i,j}\left(X_i^{e_{N_3}} - X_i^{\hat{O}}\right)\left(X_j^{e_{N_3}} - X_j^{\hat{O}}\right) + \sum_{i=1}^{n} B_i\left(X_i^{e_{N_3}} - X_i^{\hat{O}}\right)\right] < 0. \\ \vdots \qquad\qquad \vdots \qquad\qquad \vdots \\ Z_{e_{N_k}} - Z_{e_W} = \left[\sum_{i,j=1}^{n} A_{i,j}\left(X_i^{e_{N_k}} - X_i^{\hat{O}}\right)\left(X_j^{e_{N_k}} - X_j^{\hat{O}}\right) + \sum_{i=1}^{n} B_i\left(X_i^{e_{N_k}} - X_i^{\hat{O}}\right)\right] - \left[\sum_{i,j=1}^{n} A_{i,j}\left(X_i^{e_W} - X_i^{\hat{O}}\right)\left(X_j^{e_W} - X_j^{\hat{O}}\right) + \sum_{i=1}^{n} B_i\left(X_i^{e_W} - X_i^{\hat{O}}\right)\right] < 0. \end{cases} \tag{2}$$

where $A_{i,j}, B_i$, and $X_j^{\hat{O}}$ are the unknowns and $X_j^{\hat{O}}$ is bounded by the boundaries of the subregion hypothesized to contain $\hat{O}$. If previously mentioned system of quadratic inequalities does not have a feasible solution, the candidate subregion cannot contain RO and *vice versa*.

Each of the inequalities in Equation (2) compares the canonical quadratic distance between a pair of experiments, for example, *W* and *B*, to $\hat{O}$. Given that $\hat{O}$ is contained in the same sb with *W*, as the size of sb (S_{sb}) decreases, the canonical quadratic distance of *W* will be less than other experiments (with better ranks), making the system of inequalities (Equation (2)) infeasible. Because this contradicts the existence of RO in one of the subregions, the proof is complete.

The following example illustrates the previously mentioned proof using a simple two-dimensional FS.

3.4.1. Example: analysis for existence and size of an NOR subregion in a sample with two-dimensional FS. Figure 4 illustrates two-dimensional FS of unit length with seven experiments from a D-optimal design. We consider uniform grid for subregions, for example, $dx_i = \alpha$ for $i = 1, 2$. For the candidate subregion where *W* experiment resides on the northeast corner, the system of quadratic equations can be written as

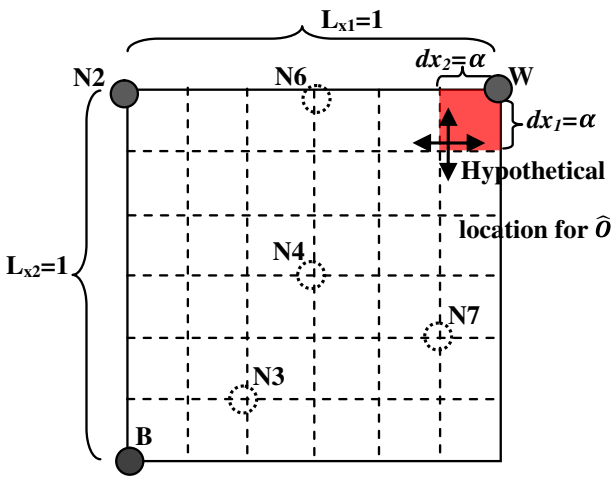


Figure 4. Two-dimensional FS with seven experiments based on D-optimal design

$$\begin{cases} \vdots \\ Z_{N_2} - Z_W = \left[A(1-\alpha)^2 + B\alpha^2 - C(1-\alpha)\alpha\right] - \alpha^2[A+B+C] < 0 \\ \vdots \end{cases} \tag{3}$$

Let us consider the comparison of *N2* and *W* to find an NOR subregion with nonzero size next to *W*. In Equation (3), because the underlying function is assumed to be convex, the signs of *A* and *B* have to be positive. However, the sign of *C* can either be positive or negative depending on the orientation of the function and the relative location of the comparing experiments (*N2* and *W*) to the hypothetical optimal point $\hat{O}$. This leads to four possible combinations shown in the second column of Table II.

As shown in the third column of Table I, there is always a positive solution for the parametric quadratic inequality $Z_{N_2} - Z_W < 0$ in Equation (3) regardless of the sign of C for *N2* and *W*. In other words, when the length (α) of the subregion next to *W* gets smaller than $\alpha_{\min} = \min\left(\frac{A}{2A+C}, \frac{+(2A-C)-\sqrt{(2A-C)^2+8AC}}{-4C}, \frac{(2A+C)+\sqrt{(2A+C)^2-8AC}}{4C}, \frac{A}{2A-C}\right)$, regardless of the location and ranking of other experiments, the inequality $Z_{N_2} - Z_W < 0$ of the Equation (3) is violated. This means, in the previously mentioned situation, the subregion next to *W* cannot contain the hypothetical optima $\hat{O}$. It should be noted that, in this example, choosing any other pair of experiments in Equation (3) other than *W* and *N2* may result in increasing (not decreasing) $\alpha_{\min}$. As proved in Theorem 1, the identification of nonzero size subregion using experiment rankings is independent of the locations of the experiments. Also as indicated in Theorem 1, the number of subregions not containing the real optimum (NORs) is at least one, that is, there can be more than one NOR.

In the following section, we develop an algorithm for eliminating subregions not containing the optimal point by using the strategy of the proof of Theorem 1.

3.5. *Reducing FS*

The reduction of the FS to a subregion containing RO is achieved through the ranking of experiments in the current run. This reduction is performed by eliminating those subregions that do not contain the optimal point, for example, NORs. The determination of such subregions is exact as per the assumption stated in Section 3.1 and Theorem 1. Using the proof of Theorem 1, the elimination process of nonoptimal subregions can be formalized in an algorithm as follows:

NOR elimination procedure

Step 1. Divide FS into k^n subregions of the same size and structure by dividing each factor into k ($n > 1$) equal size subsections using k-1 hyperplanes orthogonal to the n factor dimensions.

Step 2. For each of the k^n subregions, repeat the following:

2.1. Identify a hypothetical optimal point $\hat{O}$ in the current subregion.

2.2. For each experiment $1 \leqslant e \leqslant E$, express the response model in a canonical form as $Z_e = \sum_{i,j=1}^{n} A_{i,j}\left(X_i^e - X_i^{\hat{O}}\right)\left(X_j^e - X_j^{\hat{O}}\right) + \sum_{i=1}^{n} B_i\left(X_i^e - X_i^{\hat{O}}\right) + R^e$, where $A_{i,j} \in R$ and R^e is a constant term.

2.3. Sort the parametric canonical forms of the experiments in ascending order as $\left(Z_{e_B} < Z_{e_{N_2}} < \cdots < Z_{e_W}\right)$.

2.4. Rewrite the sorted canonical forms of the experiments in the form of a system of inequalities with $E(E-1)/2$ pairwise comparisons of experiments as in Equation (1).

2.5. Check the feasibility of the previously mentioned system by looking for a negative solution of the following min–max optimization:

$$\begin{aligned} &\text{Min Max } Z = \left(Z_{e_B} - Z_{e_{N_2}}, Z_{e_B} - Z_{e_{N_2}}, \ldots, Z_{e_{N_k}} - Z_{e_W}\right) \\ &\text{Subject to :} \\ &\qquad A_{i,j} \in R,\ X_j^{\hat{O}} \in \text{Current subregion} \end{aligned} \tag{4}$$

We note that the nonexistence of a positive solution to the optimization model in Equation (4) is equivalent to the nonexistence of a feasible solution for the system of quadratic inequalities in Equation (3) and *vice versa*. Clearly, the previously mentioned procedure eliminates only those subregions not containing the optimal point by contradicting the assumptions stated in Section 3.1. In other words, the procedure only checks the necessary condition for OR subregions. Therefore, the remaining subregions that are designated as the FS of the next run may or may not contain the optimum. Subsequently, these subregions are tested in the following runs by adding more experiments (or decreasing the size of the subregions).

Table II. Possible combinations of $Z_{N_2} - Z_W$ based on sign of interaction term (C)

No.	Possible combination	Solution
1	$[A(1-\alpha)^2 + B\alpha^2 - C(1-\alpha)\alpha] - \alpha^2[A+B+C] < 0$	$\alpha > \frac{A}{2A+C}$
2	$[A(1-\alpha)^2 + B\alpha^2 + C(1-\alpha)\alpha] - \alpha^2[A+B+C] < 0$	$\alpha > \frac{+(2A-C)-\sqrt{(2A-C)^2+8AC}}{-4C}$
3	$[A(1-\alpha)^2 + B\alpha^2 - C(1-\alpha)\alpha] - \alpha^2[A+B-C] < 0$	$\alpha > \frac{(2A+C)+\sqrt{(2A+C)^2-8AC}}{4C}$
4	$[A(1-\alpha)^2 + B\alpha^2 + C(1-\alpha)\alpha] - \alpha^2[A+B-C] < 0$	$\alpha > \frac{A}{2A-C}$

3.6. *Computational complexity and accuracy of NOR elimination procedure*

The computational complexity and accuracy of NOR elimination procedure depends on three variables, E, n, and k:

(1) E, the number of experiments, affects the number of quadratic inequalities (NIQ) in the system of quadratic inequalities by a polynomial order $\left(\text{NIQ} = \frac{E(E-1)}{2}\right)$.

(2) n, the number of dimensions, affects both the number of variables in quadratic inequalities (V) by a polynomial order $\left(V = 3\binom{n}{1} + \binom{n}{2}\right)$ and the number of procedure iterations (PI) by an exponential order ($\text{PI} = k^n$).

(3) k, the number of divisions in each FS, affects the number of the procedure iterations (PI) by an exponential order ($\text{PI} = k^n$).

As a result, the complexity of the elimination procedure grows exponentially with increasing n and k. In other words, O-ASRSM trades off between the total number of experiments and the computational complexity of the algorithm. In most practical cases, the computational effort necessary is negligible, either due to the existence of powerful computational resources (e.g. parallel computing facilities) or due to experiments being too costly *vis-à-vis* the computational effort. In other cases, the choice of k can save the computational effort considerably while keeping the accuracy of the algorithm at an acceptable level.

Typically, choosing a small k reduces the total area of the NORs eliminated from the FS. Although the elimination of the regions is exact (as long as the rankings are correct), the retained region (FS) may still contain nonoptimal subregions necessitating further experimentation and subdivision (see Section 3.4). In comparison, choosing a large k increases the total area of NORs, whereas making the elimination process is computationally more expensive as there are more subregions. Figure 5 illustrates a simulated example on the effect of two choices of k on the NOR elimination procedure results based on a two-dimensional FS with six points of the D-optimal design.

One strategy for setting k, as used in this article, is to start with a small value (e.g. $k = 4$–6) and then increase it as necessary in the subsequent runs. This strategy demonstrated promising performance in both computational time and accuracy throughout the simulated experiments.

3.7. *Parametric approach: model fitting strategy*

We use a parametric approach based on model fitting concurrent to the nonparametric ranking approach described in Section 3.3. This strategy not only allows us to increase the precision of EO_r but also supports backtracking through the expansion of OR_r to contain estimated optimal EO_r. Beginning with the completion of all first run experiments, this parametric approach is used after each experiment. In this approach, we fit a quadratic model: $Z = \sum_{i,j=1}^{n} Q_{i,j} x_i x_j + \sum_{i=1}^{n} P_i x_i + R + \varepsilon$, with $\varepsilon \sim N(0, \sigma^2)$, using all the experimental data as they are accumulated to analyze the underlying function and efficacy of conducted experiments. In fitting the quadratic model, the main objective is to find the estimated optimal experiment (EO_r). EO_r, the minimum of the fitted model, shows the predicted optimal solution. Furthermore, the change in the EO_r in consecutive runs is also used as a stopping criterion. It should be noted that instead of EO_r, calculating the adjusted coefficient of determination $\left(R^2_{\text{adj}}\right)$ may also be incorporated. R^2_{adj} shows how well the information gained from the experiments explain the behavior of the underlying system.[56] In this article, we use R^2_{adj} only to compare the performance of the proposed methodology with other approaches from the literature.

3.8. *Selecting additional points*

When the model fitting strategy terminates without satisfying the convergence criteria, then additional points are needed. An additional point can be selected one at a time or simultaneously to exploit the parallel experimentation capability. However, as will be discussed shortly, we recommend the addition of only one point at a time to keep the total number of experiments as small as possible. Additional points not only improve the accuracy of the model fitting strategy but also enable eliminating more of the subregions in several ways. First, they increase the number of pairwise ranking comparisons of experiments such that the likelihood of a previously noneliminated

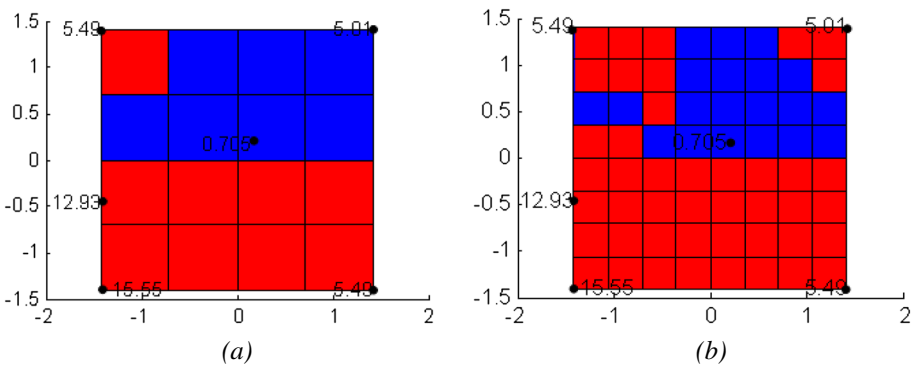


Figure 5. The effect of subregion size on the NOR elimination procedure results: (a) 64 subregions of a two-dimensional FS; (b)16 subregions of a two-dimensional FS. The FS is defined as $\{(X, Y) | (X, Y) \in [-1.4142, 1.4142]\}$. ORs and NORs are highlighted with blue and red, respectively

subregion becoming a NOR is increased. Second, with these additional points, the new ranking of the experiments leads to a better coverage of FS. Finally, additional points result in more reliable ranking of the experiments when the underlying function is noisy. The necessary condition for the above claims is that the additional points do not change the characterization of previously labeled NOR subregion, which can be proven when the underlying function is convex quadratic and deterministic. The following proposition guarantees the consistent characterization of the NOR through adding additional points:

Proposition 1:
If the underlying function is convex quadratic and without noise, then the addition of experiment(s) to the *r*th run FS does not reduce the size of the NORs identified in the $((r-1)$th run.

Proof
Let E denote the number of experiments at the $(r-1)$th run where the FS (FS_{r-1}) has been divided into k^n subregions. The necessary condition for optimality of each subregion is the feasible solution of the system of Equation (1), consisting of $E(E-1)/2$ inequalities at the $(r-1)$th run. Adding F new experiments to the design in the next run (r) will add $(E+F)(E+F-1)/2 - E(E-1)/2$ inequalities to Equation (1) for each subregion while preserving the previous inequalities. This addition of constraints only reduces the feasible space of Equation (1), which clearly does not cause NORs to become ORs. Therefore, the addition of point(s) to the FS in a run will not reduce the size of the previous run's NORs. □

Corollary 1:
If the underlying function is convex quadratic and without noise, then NORs and ORs across NOR elimination procedures are nondecreasing and nonincreasing sets, respectively.

Proof
On the basis of Proposition 1, additional experiments do not decrease the NORs. Therefore, moving from one run to the next, by potentially including additional runs, NORs will not decrease or equivalently ORs are nonincreasing.

Corollary 1 shows that the FS area can be reduced toward the optimal point by adding more experiments. However, because one of the goals of O-ASRSM is to reduce the total number of experiments, the number of additional points (E^*) should be kept as small as possible, preferably by adding one at a time. For this purpose, each of the additional points can be selected by implementing an augmented optimal design with E^* experiments (in this study we use $E^*=1$) on the remaining parts of FS_{r-1}, after eliminating the NORs ($OR_{r-1} = FS_r$). Augmentation of the optimal design D with respect to OR_{r-1} can be performed by adding a total of $m \times 2^n$ constraints, where m is the number of NORs and n is the number of factors, to the objective function of the optimal design. Each set of 2^n constraints is for turning one of NORs to unfeasible parts of FS_r, where each constraint can be written as

$$\prod_{i=1}^{n} \frac{\max[(X_i - X_{i_L}), 0]}{(X_i - X_{i_L})} \times \frac{\max[(X_{i_U} - X_i), 0]}{(X_{i_U} - X_i)} = 0 \tag{5}$$

In Equation (5), (X_{i_L}, X_{i_U}) are the lower and upper bounds of the selected NOR subregion. The denominators in Equation (5) are used for scaling purposes such that the left-hand side of the equation becomes either 0 or 1. Note that this approach could also be used to tackle simple bound constraints within the O-ASRSM method, thereby making it applicable to a broader range of engineering design problems, for example, constrained problems with simple bound constraints.

The optimization model (Equation (6)) exemplifies the D-optimal objective function as well as the constraints imposed by the NORs for the example discussed in Section 3.6 (Figure 5a). The first constraint in Equation (6) checks if a point in the FS is contained in the small NOR on the upper left part of FS (highlighted with red in Figure 5a). Similarly, the second constraint checks if a point in the FS is contained in the large NOR on the lower half of FS in Figure 5b. Each of the four elements on the left-hand side of the first and second constraints identifies one side of the NORs' boundaries. For example, $\max[(X-(-1.4142)),0]$ corresponds to the right side of boundary at $X=-1.4142$ in both first and second constraints:

$$\begin{aligned} &\text{Min } Z = \left|\left(X'X\right)^{-1}\right| \\ &s.t. \\ &\frac{\max[(X-(-1.4142)),0]}{(X-(-1.4142))} \times \frac{\max[(Y-\!\!-0.7071),0]}{(Y-\!\!-0.7071)} \times \frac{\min[(X-(-0.7071)),0]}{(X-(-0.7071))} \times \frac{\min[(Y-1.4142),0]}{(Y-1.4142)} = 0 \\ &\frac{\max[(X-(-1.4142)),0]}{(X-(-1.4142))} \times \frac{\max[(Y-\!\!-(-1.4142)),0]}{(Y-\!\!-(-1.4142))} \times \frac{\min[(X-1.4142),0]}{(X-1.4142)} \times \frac{\min[(Y-0),0]}{(Y-0)} = 0 \end{aligned} \tag{6}$$

4. Numerical examples

In this section, we describe two sets of simulated experiments performed to evaluate the performance of the proposed O-ASRSM approach. In the first set of simulations O-ASRSM is compared with the well-known methods including CCD, BBD and A-, D-, and

V-optimal designs using different quadratic response models with varying variance of errors. The second set of simulations study the performance of the proposed approach along with classical models, optimal designs and two global optimization methods (Standler *et al*.[23] Wang[22]) on several nonlinear response models with varying levels of noise.

4.1. *Quadratic response models*

We now describe the simulated experiments performed to compare the performance of the proposed O-ASRSM approach with those of CCD, BBD, A-, D-, and V-optimal designs on quadratic response models. In the simulated experiments, we have considered three response models with two variables, two models with three variables, and two models with six variables all with different levels of error variance and quadratic function types (i.e. convex and nonconvex). These response models are presented in Table III. As noted earlier, all response models considered in this section have a quadratic relation with a normal error term $\varepsilon \sim N(0, \sigma^2)$. Figure 6 shows the contour plots of the first and second responses.

The O-ASRSM is an adaptive sequential method, whereas the CCD, BBD, A-, D-, and V-optimal designs are essentially preset designs. To evaluate the effect of this difference, we initially fixed the number of design points at 7 for cases with two variables, 11 for cases with three variables, and 34 for cases with six variables and then incrementally added two more design points one at a time. For optimal designs, the initial set of design points is optimally generated by optimizing the optimality criteria over the starting FS with a fine grid system spaced with 0.01 intervals. Next, each of the additional points is generated by optimizing the optimality criterion given the existing design points and the response model. For the CCD and BBD, we initially used 7, 11, or 34 experiments of the full design by excluding some of the points and then reincluding them one at a time. For fair comparison, the location of additional points in CCD and BBD is chosen based on their closeness to the direction of maximum improvement.

The performance metrics used are average R^2_{adj}, average optimality gap (i.e. deviation from the optimal response), and sum of squared errors in estimating the original function. All simulated experiments are repeated four times, and average results are reported. The starting FS expands the initial region of interest, by a factor of 1.4142 in both directions for the cases with two variables, by a factor of 1.6817 in related directions for the cases with three variables, and by a factor of 2.3784 in all directions for the cases with six variables. This expansion is performed to account for the axial points. Table IV presents the average R^2_{adj} performances for

Table III. Quadratic response models used in the simulated experiments

No. variables	Experiment no.	Response relation	Error (ε)	Response type
Two-variable response	1.1	$W = -2x^2 + 3y^2 + 2x - y + 2xy - 1 + \varepsilon$	N (0,0.1)	Nonconvex
	1.2	$W = x^2 + 2y^2 - 2y + \varepsilon$	N (0,1)	Convex
	1.3	$W = -2x^2 + 3y^2 + 2x - y + 2xy - 1 + \varepsilon$	N (0,2)	Nonconvex
Three-variable response	2.1	$W = 2\,x^2 - 1y^2 - 2z^2 + x - 2y + 3z - xy + 3xz + 2yz + 2 + \varepsilon$	N (0,2)	Nonconvex
	2.2	$W = -1.5\,x^2 - 3.5y^2 + 3z^2 + 0.5x - 3.5y - 1.5z - 3xy + 1.3xz + 1.4yz + 2 + \varepsilon$	N (0,2.5)	Nonconvex
Six-variable response	3.1	$W = (t - 0.55)^2 + (u + 0.7)^2 + (v - 0.33)^2 + (x - 1.55)^2 + (y + 0.9)^2 + (z - 0.3)^2$	N (0,2)	Convex
	3.2	$W = (t - 1.65)^2 + (u + 1.7)^2 + (v - 1.45)^2 + (x - 2.11)^2 + (y + 1.91)^2 + (z - 2.01)^2 + (t - 2)(u - 2.2) + (u - 1.54)(v - 0.02) + (u - 0.34)(z - 2.33) + (v - 0.34)(y - 1.33) + (y - 0.53)(z - .65)$	N (0,1)	Convex

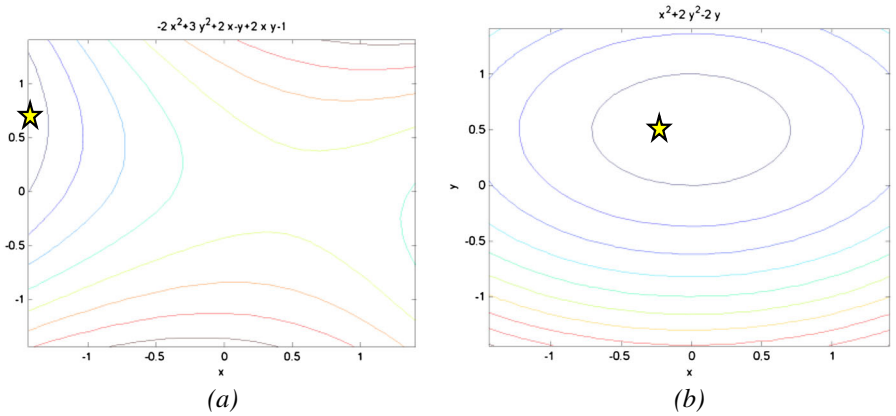


Figure 6. Contour plot of the responses 1.1 and 1.2 in Table II (stars indicate the locations of optimum)

Table IV. R^2_{adj} for trials 7, 8, and 9 of the quadratic responses with two variables; trials 11,12, and 13 of the quadratic responses with three variables; and trials 34, 35 and 36 of the quadratic responses with six variables

		Adjusted R^2					
Experiment no.	No. observation	CCD	BBD	O-ASRSM	D-optimal	V-optimal	A-optimal
1.1	7	99.96%	N/A	99.99%	99.96%	99.92%	99.94%
	8	99.96%	N/A	99.99%	99.98%	99.95%	99.95%
	9	99.95%	N/A	99.99%	99.97%	99.94%	99.92%
1.2	7	92.69%	N/A	98.74%	95.01%	94.85%	90.69%
	8	92.48%	N/A	98.42%	89.20%	95.86%	86.86%
	9	92.00%	N/A	97.15%	90.42%	95.42%	86.58%
1.3	7	69.77%	N/A	92.95%	92.96%	72.11%	97.71%
	8	70.60%	N/A	94.59%	91.06%	74.92%	79.86%
	9	88.48%	N/A	95.55%	89.02%	80.89%	82.00%
Ave.	7	87.47%	N/A	97.23%	95.98%	88.96%	96.11%
	8	87.68%	N/A	97.67%	93.41%	90.24%	88.89%
	9	93.48%	N/A	97.56%	93.14%	92.08%	89.50%
2.1	11	87.30%	76.11%	93.13%	98.18%	92.66%	98.42%
	12	88.10%	81.32%	96.29%	98.61%	95.60%	96.60%
	13	91.09%	79.87%	98.32%	97.66%	95.67%	97.79%
2.2	11	89.02%	53.12%	98.39%	89.25%	84.88%	90.50%
	12	87.06%	56.04%	97.37%	92.93%	86.88%	91.76%
	13	86.50%	49.48%	95.36%	91.74%	88.27%	90.12%
Average	11	88.16%	64.62%	95.76%	93.72%	88.77%	94.46%
	12	87.58%	68.68%	96.83%	95.77%	91.24%	94.18%
	13	88.80%	64.68%	96.84%	94.70%	91.97%	93.96%
3.1	34	80.21%	70.00%	98.63%	90.20%	96.49%	90.20%
	35	79.61%	70.10%	98.94%	91.84%	96.76%	91.84%
	36	79.82%	64.18%	99.05%	92.73%	97.26%	92.73%
3.2	34	99.56%	98.27%	99.92%	97.80%	99.93%	99.82%
	35	99.55%	98.27%	99.94%	99.81%	99.94%	99.85%
	36	99.55%	98.27%	99.95%	99.82%	99.94%	99.81%
	34	89.89%	84.14%	99.28%	94.00%	98.21%	95.01%
Average	35	89.58%	84.19%	99.44%	95.83%	98.35%	95.85%
	36	89.69%	81.23%	99.50%	96.28%	98.60%	96.27%

consecutive trials. Figures 7a and 7b illustrate the average R^2_{adj} of the estimated response surfaces for Experiments 1.1–1.3, 2.1 and 2.2, and 3.1 and 3.2.

Table IV and Figure 7 show that the O-ASRSM is competitive in R^2_{adj} performance with the rest of the methods. In particular, when the number of experiments is limited, O-ASRSM is consistently the best method in terms of R^2_{adj}. Table V presents the optimality gap results of the consecutive trials of the comparing methods. The optimality gap is measured as the deviation of the response at the

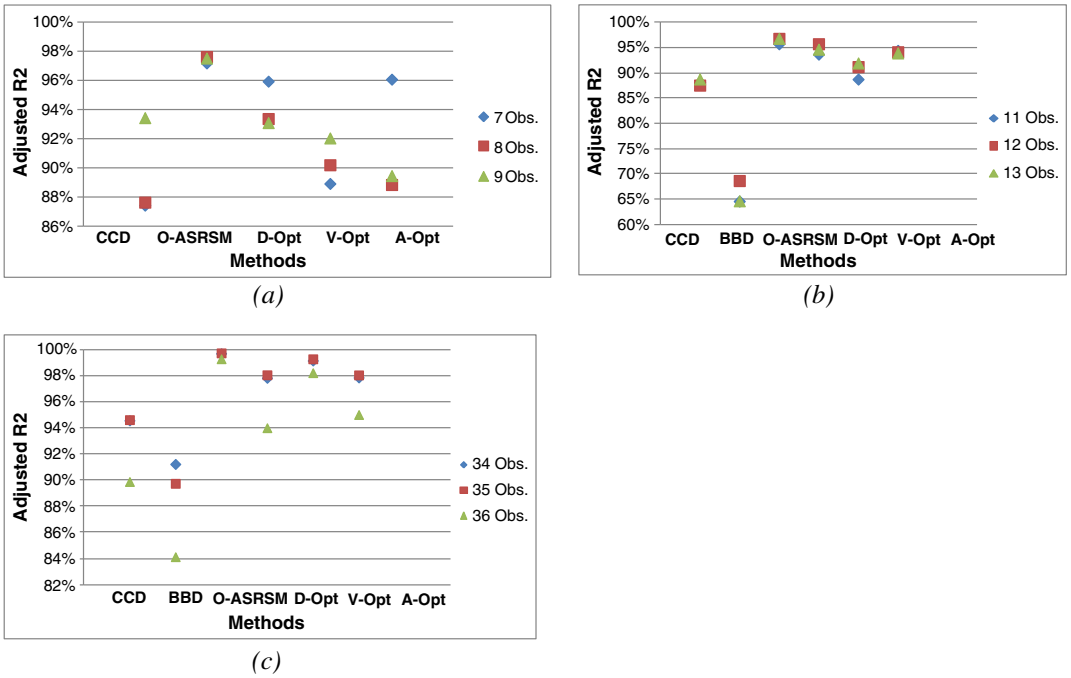


Figure 7. Comparison of the average R^2_{adj} performance of the studied methods: (a) Experiments 1.1 to 1.3 (two variables), (b) Experiments 2.1 to 2.3 (three variables), and (c) Experiments 3.1 to 3.2

Table V. Optimality gap for trials 7, 8, and 9 of the quadratic responses with two variables; trials 11,12, and 13 of the quadratic responses with three variables; and trials 34,35, and 36 of the quadratic responses with six variables

		Optimality gap					
Experiment no.	No. observation	CCD	BBD	O-ASRSM	D-optimal	V-optimal	A-optimal
1.1	7	3.84	N/A	0.00	0.00	31.76	0.00
	8	3.84	N/A	0.00	0.00	18.35	4.70
	9	0.23	N/A	0.00	0.26	0.00	0.00
1.2	7	70.52	N/A	0.07	0.00	0.61	40.19
	8	70.52	N/A	0.06	0.53	0.76	29.94
	9	70.52	N/A	0.01	7.69	0.83	8.24
1.3	7	909.82	N/A	0.23	0.31	0.31	1260.68
	8	909.82	N/A	0.25	0.31	0.31	492.09
	9	909.82	N/A	0.30	0.31	0.31	5.02
2.1	11	19.24	18.99	12.08	11.95	13.84	13.5
	12	19.46	19.02	9.75	10.88	13.84	12.66
	13	13.09	19.42	8.02	10.56	14.01	11.81
2.2	11	19.3	20.28	2.51	6.39	1.4	1.43
	12	19.3	20.64	1.02	6.37	1.37	1.41
	13	19.53	19.75	1.06	6.4	1.39	1.43
3.1	34	3.94	2.06	0.57	0.46	0.17	0.46
	35	6.65	2.00	0.17	0.17	0.23	0.17
	36	6.67	4.20	0.15	0.19	0.23	0.19
3.2	34	4.94	4.24	0.06	0.19	0.09	0.04
	35	4.63	4.24	0.04	0.07	0.09	0.04
	36	4.63	4.24	0.02	0.07	0.05	0.03

final EO from the response at true optimal experiment RO. Figure 8 also illustrates a graphical representation of the shrinking process of the FS using O-ASRSM for the response in Experiment 1.3. The experiments show that the optimality gap of the proposed O-ASRSM is the most competitive among all methods. Figure 9 illustrates the performances across all models for their last trial. The performance of O-ASRSM for higher order factor experiments is consistent with that of lower order response models, indicating its robustness with increasing number of factors.

4.2. *Nonlinear response models*

In this set of experiments, we compare the performance of the proposed O-ASRSM approach with two global optimization methods (e.g. Standler *et al.*[23] and Wang[22]) as well as with the classical CCD, BBD, and optimal designs (A-, D-, and V-optimal). We used seven nonlinear response models with two, three, and six variables and varying variance of error and function type. These response models are presented in Table VI (see also Figure 10).

For analysis, we studied the performances based on the average optimality gap and the Euclidian distance of the estimated optima to the real optimal point. All simulated experiments are repeated three times, and average results are reported. As in the preceding section, we report the results of trials 7, 8, and 9 for the cases with two variables; trials 11, 12, and 13 for the cases with three variables; and trials 34, 35, and 36 for the cases with six variables. Table VII shows the average optimality gap results of the consecutive trials of the alternative methods. Figure 11 also illustrates the shrinking process of the FS using O-ASRSM for the second response function.

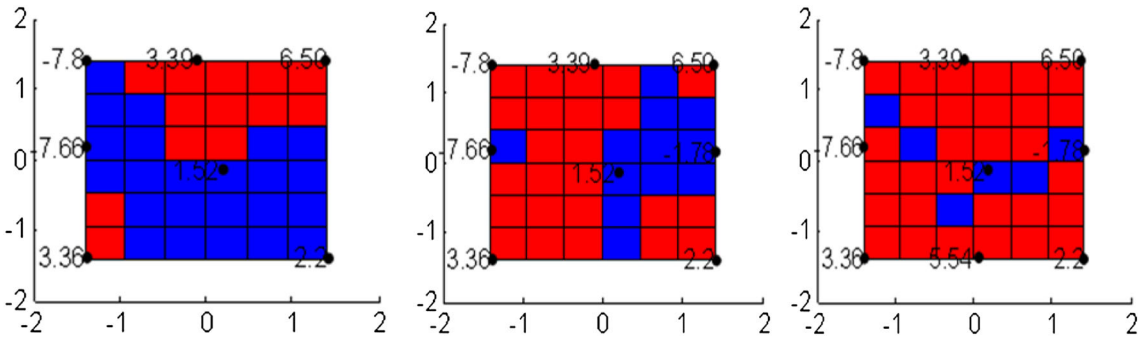
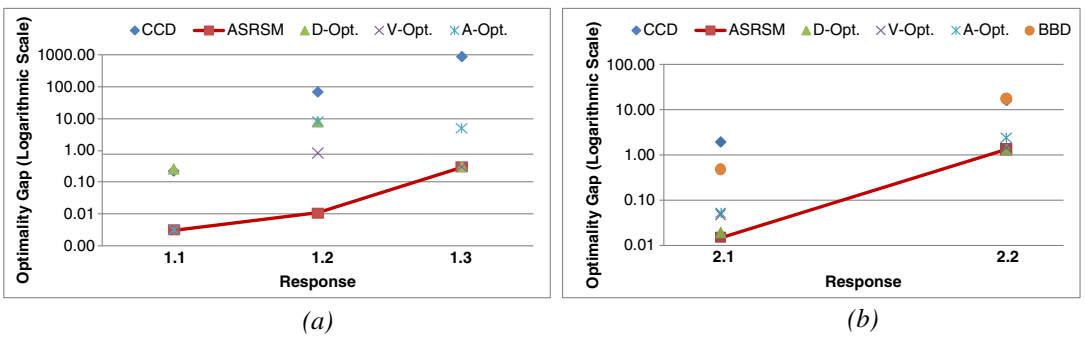


Figure 8. Graphical representation of the shrinking process of the FS using O-ASRSM for the response in Experiment 1.3 (a–c). Blue and red colors indicate that the sub-region is an OR and NOR, respectively



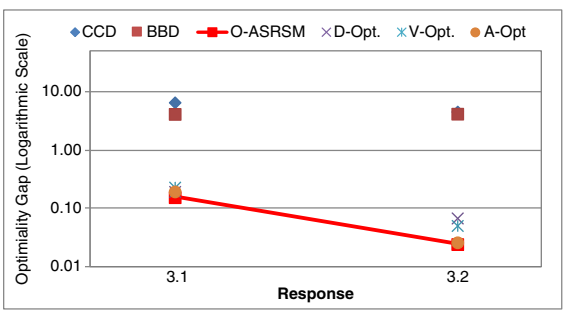


Figure 9. The optimality gap of the last trial: (a) experiments with two variables, (b) experiments with three variables, and (c) experiments with six variables

Table VI. Nonlinear response models used in the simulated experiments

No. variables	Experiment no.	Response relation	Error
Two-variable response	1.1	$W = y - \left(\frac{1}{8\pi^2}x^2\right) + \left(\frac{10}{\pi}\right)(x-2)^2 + 10\left(3 - \frac{1}{12\pi}\right)\cos(x) + \varepsilon$	N (0,3.5)
	1.2	$W = 0.75(x-0.15)^2 + 0.25(x-0.15)^4 + 1.3(x-0.15)^6 + 1.8(x-0.15)(y-1)^2 - 2.66\,(y-1)^2 + 1.9(y-0.15)^2 + \varepsilon$	N (0,2)
Three-variable response	2.1	$W = (x-0.55)^2 + (y+0.7)^2 + (z-0.33)^2 - \cos(18(x-0.55)) - \cos(18(y+0.7)) - \cos(18(z-0.33)) + \varepsilon$	N (0,2)
	2.2	$W = (x-1)^3 - 3(y-1)^3 + (z+1)^3 - 2(x-1)^2 - 2(y-1)^2 + (z+1)^2 - (x-1) + 5(y-1) + 6(z+1) + 2(x-1)(y-1) + (x-1)(z+1) - 4(y-1)(z+1) + 1 + \varepsilon$	N (0,1)
	2.3	$W = x^2 + \exp\left(\frac{y}{10} + 10\right) + \sin(zy) + \varepsilon$	N (0,3)
Six-variable response	3.1	$W = 6.6(t-2)^4(u-1.1)^2 + \frac{3.6(v-1.35)^6}{((x-2.3)^2+1)} + 1.5(x-2.3)(y-1.1)^2(z-0.25)^4$	N (0,2)
	3.2	$W = -\exp(-1(10(t-0.1312)^2 + 3(u+0.1696)^2 + 17(v-0.5569)^2 + 3.5(x-0.0124)^2 + 1.7*(y+0.8283)^2 + 8(z-0.5886)^2)) - \exp(-1(.05(t-0.2329)^2 + 10(u+0.4135)^2 + 17(v-0.8307)^2 + 0.1(x-0.3736)^2 + 0.8(y+0.1004)^2 + 14(z-0.9919)^2))$	N (0,1)

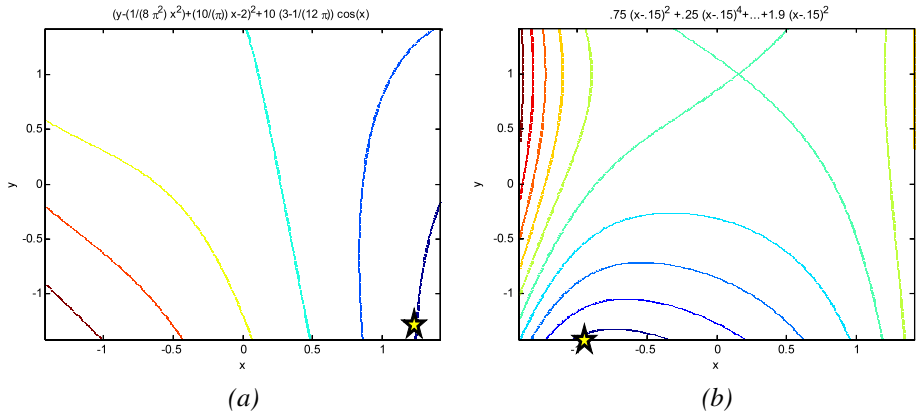


Figure 10. Contour plots of the responses 1.1 and 1.2 in Table V (stars indicate the location of optimum)

Table VIII shows the average Euclidean distance of the estimated optima to the real optima of the underlying function for different methods. Interestingly, the comparison of results in Tables VII and VIII reveals that some of the estimated optima (EOs) that are further away from the real optima (ROs) attain better responses than those EOs closer to the ROs. Our subsequent analyses indicate that while some EOs can be further away from ROs, they attain better average response due to curvature variation of the response around the RO. These results also indicate that, as in quadratic responses, the O-ASRSM's performance is robust with respect to the increasing number of factors.

5. Conclusions

An adaptive methodology for response surface optimization is developed and presented. By combining concepts from the optimal design of experiments, nonlinear optimization, and RSM, the O-ASRSM improves the experimentation efficiency, for a given response target by identifying the input factor combination (or containing region) in a smaller number of experiments than the classical single-shot RSM designs. This sequential adaptive experimentation approach uses the information gained from previous experiments to design the subsequent experiment while simultaneously reducing the region of interest and identifying factor combinations for new experiments. The distinct features are its optimality (under certain assumptions), inheritance of results from previous experiments, and robustness due to experiment ranking based reduction of the region of interest. On the basis of the results of extensive simulated experiments, it is shown that O-ASRSM outperforms the popular CCD, BBD, and optimal designs in terms optimality for quadratic responses. Furthermore, the O-ASRSM is very competitive in comparison with the alternative approaches in estimating the optima of nonlinear responses. Future extensions of the proposed method include considering higher order of response functions and mixed FSs with discrete and continuous factors.

Table VII. Optimality gap for trials 7, 8, and 9 of the nonlinear responses with two variables; trials 11,12, and 13 of the nonlinear responses with three variables; and trials 34, 35, and 36 of the nonlinear responses with six variables

		Optimality gap							
Experiment no.	Run	CCD	BBD	O-ASRSM	Standler *et al.*[23]	Wang[22]	D-optimal	A-optimal	V-Optimal
1.1	7	438.43	N/A	0.07	0.03	633.55	0.01	0.1	0
	8	174.6	N/A	0.01	668.52	403.37	0	0.1	0
	9	0.02	N/A	0	668.24	917.63	0.04	1.18	0.01
1.2	7	964.35	N/A	4.78	6.27	226.22	171.41	3.1	13.44
	8	436.18	N/A	3.52	589.92	383.74	181.93	5.18	4.55
	9	5.32	N/A	4.75	982.38	197.61	182.05	5.56	6.7
2.1	11	35.26	81.08	14.79	13.64	39.95	10.08	14.75	18.97
	12	32.03	17.07	5.47	97.05	11.51	16.2	13.62	14.6
	13	89.84	24.54	2.86	105.9	12.77	28.89	13.44	18.24
2.2	11	161.85	299.34	5.88	6.20	194.53	1.58	6.91	2.13
	12	71.22	31.8	2.17	92.97	21.67	2.68	7.55	3.57
	13	120.27	4.06	2.04	151.54	0.03	2.83	6.66	35.41
2.3	11	1.90E + 07	3.20E + 07	2.01E + 07	7.90E + 06	1.90E + 07	3.10E + 07	2.90E + 07	3.10E + 07
	12	5.20E + 07	3.20E + 07	0.67	1.10E + 07	0.71	3.10E + 07	2.90E + 07	3.00E + 07
	13	2.10E + 07	2.10E + 07	0.39	1.10E + 07	0.4	3.20E + 07	2.90E + 07	3.10E + 07
3.1	34	295.76	300.76	223.96	282.53	242.07	245.62	240.49	213.44
	35	296.69	290.56	143.67	285.79	241.74	241.00	240.47	107.87
	36	296.69	290.57	106.18	293.37	232.28	245.01	240.47	121.31
3.2	34	1.67	1.64	0.99	1.42	1.01	0.98	1.02	0.98
	35	1.41	1.65	0.91	1.76	1.05	0.98	0.96	0.96
	36	1.52	1.52	0.87	1.82	0.95	0.97	0.98	0.96

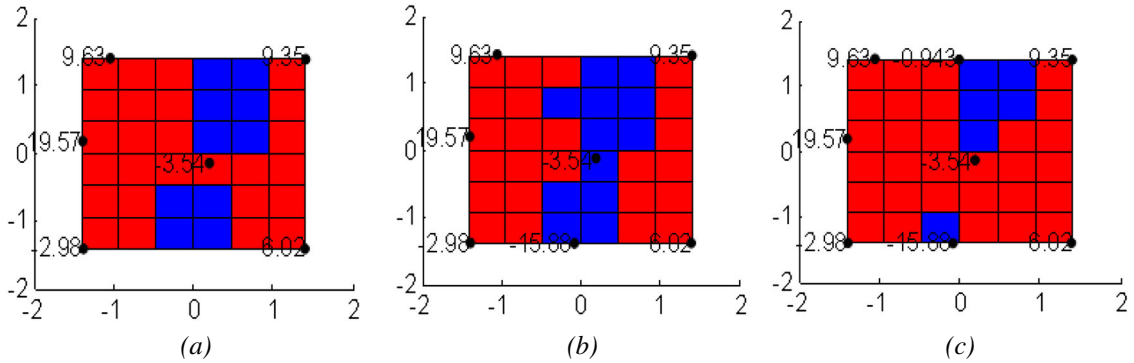


Figure 11. Graphical representation of the shrinking process of the FS using O-ASRSM for response 1.2. Blue and red colors indicate that the subregion is an OR and NOR, respectively

Table VIII. The average Euclidian distance to the optimum for trials 7, 8, and 9 of the nonlinear responses with two variables; trials 11,12, and 13 of the nonlinear responses with three variables; and trials 34, 35, and 36 of the nonlinear responses with six variables

		Euclidean distance to the optimum							
Experiment no.	Run	CCD	BBD	O-ASRSM	Standler *et al.*[23]	Wang[22]	D-optimal	A-optimal	V-optimal
1.1	7	2.43	N/A	0.26	0.05	1.84	0.09	0.31	**0.01**
	8	1.65	N/A	**0**	3.17	2.56	**0**	0.32	**0**
	9	0.13	N/A	0.05	3.17	3.01	0.19	1.09	**0.01**
1.2	7	3.01	N/A	0.45	0.51	0.96	1.11	**0.39**	0.58
	8	1.97	N/A	**0.42**	2.02	2.2	1.17	0.46	0.44
	9	0.45	N/A	**0.43**	2.39	1.73	1.17	0.47	0.5
2.1	11	1.09	2.18	**0.3**	0.42	1.2	0.31	0.83	1.09
	12	1.06	1.3	**0.69**	2.01	0.38	1.02	0.89	1.37
	13	1.53	0.62	0.43	2.25	**0.32**	1.21	0.97	1.11
2.2	11	2.02	2.69	0.7	0.9	1.95	**0.54**	0.55	0.79
	12	1.34	0.99	**0.57**	3.33	0.69	0.6	0.66	0.81
	13	1.07	0.46	0.53	3.87	**0.19**	0.58	0.86	0.77
2.3	11	0.48	1.76	0.48	0.32	3.21	**0.63**	0.47	0.67
	12	2.23	1.59	**0.2**	2.95	0.39	0.7	0.41	0.74
	13	2.06	0.88	**0.15**	3.12	0.7	0.7	0.39	0.34
3.1	34	8.56	8.06	5.91	8.45	**5.12**	5.29	5.86	5.13
	35	8.31	8.78	**4.09**	8.01	5.09	5.17	5.87	4.88
	36	8.30	8.75	**4.03**	8.70	4.96	5.20	5.87	4.99
3.2	34	6.40	6.64	5.43	6.34	5.10	**5.02**	6.00	5.73
	35	6.64	6.63	**4.06**	6.84	5.21	4.92	5.98	5.73
	36	6.37	6.64	**3.54**	6.98	4.93	4.96	5.96	5.73

References

1. Box GEP, Wilson KB. On the experimental attainment of optimum conditions. *Journal of the Royal Statistical Society* 1951; **13**:1–15.
2. Gramacy RB, Lee HKH. Adaptive design and analysis of supercomputer experiments. *Technometics* 2009; **51**(2):130–145.
3. Gu L. A comparison of polynomial based regression models in vehicle safety analysis. In *American Society of Mechanical Engineers Design Engineering Technical Conferences—Design Automation Conference*, A. Diaz (ed.). American Society of Mechanical Engineers: New York, 2001; Paper No. DETC2001/DAC-21063.
4. Sanchez SM, Sanchez PJ. Very large fractional factorial and central composite designs. *ACM Transactions on Modeling and Computer Simulation (TOMACS)* 2005; **15**(4):362–377.
5. Box GEP, Behnken DW. Some new three level design for the study of quantitative variables. *Technometrics* 1960; **2**:455–476.
6. Myers RH, Khuri AI, Carter WH. Response surface methodology 1966–1988. *Technometrics* 1989; **31**:137–157.
7. Myers RH. Response surface methodology- current status and future directions. *Journal of Quality Technology* 1999; **31**:30–44.
8. Myers RH, Montgomery DC, Vining CG, Borror CM, Kowalski SM. Response surface methodology: a retrospective and literature survey. *Journal of Quality Technology* 2004; **36**:53–77.
9. Montgomery DC. *Design and Analysis of Experiments*, 7th Ed. John Wiley& Sons: NJ, 2008.
10. Myers RH, Montgomery DC, Anderson-Cook CM. *Response surface methodology: process and product optimization using designed experiments*, Third edition. Wiley: New York, 2009.

11. Box GEP. Statistics as a catalyst to learning by scientific method: Part II – A discussion. *Journal of Quality Technology* 1999; **31**(1):16–29.
12. Box GEP. Evolutionary operation: A method for increasing industrial productivity. *Applied Statistics* 1957; **6**:81–101.
13. Box GEP, Draper NR. *Evolutionary operation: A method for increasing industrial productivity*. John Wiley and Sons: NY, 1969.
14. Spendley GR, Hex GR, Himsworth FR. Sequential application of simplex designs in optimization and evolutionary operation. *Technometrics* 1962; **4**:441–461.
15. Friedman M, Savage LJ. Planning experiments seeking maxima. In *Techniques of Statistical Analysis*, C. Eisenhart, M. Hastay, W. A. Wallis (eds.). McGraw-Hill: NY, 1947; 363–72.
16. 0Box GEP, Hunter WG, Hunter JS. *Statistics for experimenters: design, innovation, and discovery*, 2nd Edition. Wiley Series in Probability and Mathematical Statistics: NY, 2005.
17. Czitrom V. One-factor-at-a-time versus designed experiments. *The American Statistician* 1999; **53**(2):126–131.
18. Frey DD, Engelhardt F, Greitzer EM. A Role for one factor at a time experimentation in parameter design. *Research in Engineering Design* 2003; **14**:65–74.
19. Frey DD, Jugulum R. The mechanisms by which adaptive one-factor-at-a-time experimentation leads to improvement. *American Society of Mechanical Engineers Journal of Mechanical Design* 2006; **128**:1050–1060.
20. Frey DD, Wang H. Adaptive one-factor-at-a-time experimentation and expected value of improvement. *Technometrics* 2006; **48**(3):418–31.
21. Wang G, Dong Z, Aitchison P. Adaptive response surface method - a global optimization scheme for computation-intensive design problems. *Journal of Engineering Optimization* 2001; **33**(6):707–734.
22. Wang G. Adaptive response surface method using inherited Latin hypercube designs. *American Society of Mechanical Engineers Journal of Mechanical Design* 2003; **125**(2):210–220.
23. Standler N. The Successive response surface method applied to sheet-metal forming. *Proceedings of the First MIT Conference on Computationa Fluid and Solid Mechanics*, Boston, June 12–14, 2001. Elsevier Science Ltd.: Oxford, 2001.
24. Moore AW, Schneider JM, Boyan J, Lee MS. Q2: A memory based active learning algorithm for black box noisy optimization. *Proceedings of the Fifteenth International Conference on Machine Learning*. Morgan Kaufmann, 1998; 386–394.
25. Anderson BS, Moore AW, Cohn D. A non-parametric approach to noisy and costly optimization. *Proceedings of the Seventeenth International Conference on Machine Learning (ICML)*, Santa Clara, CA, USA, 2000.
26. Alaeddini A, Yang K., Murat A. ASRSM: A Sequential Experimental Design for Response Surface Optimization. *Quality and Reliability Engineering International* 2012; To appear. DOI: 10.1002/qre.1306.
27. Sobieszczanski-Sobieski J. Optimization by decomposition: a step from hierarchic to nonhierarchic systems. *Second NASA/Air Force Symposium on Recent Advances in Multidisciplinary Analysis and Optimization*, Hampton, VA, NASA CP-3031, Part 1. Also NASA TM-101494, 1988.
28. Renaud JE, Gabriele GA. Approximation in non-hierarchic system optimization. *American Institute of Aeronautics and Astronautics Journal* 1994; **32** (1):198–205.
29. Rodriguez JF, Renaud JE, Watson LT. Convergence of trust region augmented Lagrangian methods using variable fidelity approximation data. *Structural and Multidisciplinary Optimization* 1998; **15**:141–156.
30. Jones DR, Schonlau M, Welch WJ. Efficient global optimization of expensive black-box functions. *Journal of Global Optimization* 1998; **13**:455–492.
31. Alexandrov NM, Dennis JE, Lewis RM, Torczon V. A trust-region framework for managing the use of approximation models in optimization. *Structural and Multidisciplinary Optimization* 1998; **15**(1):16–23.
32. Chang K-H, Hong J, Wan H. Stochastic trust-region response-surface method (STRONG) -- a new response-surface framework for simulation optimization. *INFORMS Journal on Computing* 2012; To appear.
33. Gano SE, Renaud JE. Variable fidelity optimization using a Kriging based scaling function. *10th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference*, Albany, New York, 2004.
34. Rodriguez JF, Perez VM, Padmanabhan D, Renaud JE. Sequential approximate optimization using variable fidelity response surface approximations. *Structural Optimization* 2001; **22**(1):24–34.
35. Baumert S, Smith RL. Pure random search for noisy objective functions, University of Michigan Technical Report, 2001.
36. Jones DR. A taxonomy of global optimization methods based on response surfaces. *Journal of Global Optimization* 2001; **21**(4):345–383.
37. Sobieszczanski-Sobieski J, Haftka RT. Multidisciplinary aerospace design optimization: survey of recent developments. *Structural and Multidisciplinary Optimization* 1997; **14**(1):1–23.
38. Kleijnen JPC. *Design and Analysis of Simulation Experiments*. Springer: New York, 2008.
39. Kleijnen JPC, Van Beers WCM, Van Nieuwenhuyse I. Constrained optimization in simulation: A novel approach. *European Journal of Operational Research* 2010; **202**(1):164–174.
40. Simpson TW, Booker AJ, Ghosh D, Giunta AA, Koch PN, Yang RJ. Approximation methods in multidisciplinary analysis and optimization: a panel discussion. *Structural and Multidisciplinary Optimization* 2004; **27**(5):302–313.
41. Chen VCP, Tsui KL, Barton RR, Meckesheimer M. A review on design, modeling and applications of computer experiments. *IIE Transactions* 2006; **38**:273–291.
42. Kiefer J. Optimum Experimental Designs. *Journal of Royal Statistical Society B* 1959; **21**:272–304.
43. Kiefer J. Optimum Designs in Regression Problems. *Annals of Mathematical Statistics* 1961; **32**:298–325.
44. Kiefer J., Wolfowitz J. Optimum Designs in Regression Problems. *Annals of Mathematical Statistics* 1959; **30**:271–294.
45. Atkinson AC, Donev AN, Tobias RD. *Optimum experimental designs with SAS*. Oxford University Press: Oxford, UK, 2007; 511+xvi. ISBN: 978-0-19-929660-6.
46. Pukelsheim F. *Optimal Design of Experiments*. Society for Industrial and Applied Mathematics (SIAM): Philadelphia, PA, 2006.
47. Andere-Rendon J, Montgomery DC, Rollier DA. Design of mixture experiments using Bayesian D-optimality. *Journal of Quality Technology* 1997; **29** (4):451–463.
48. Ginsburg H, Ben-Gal I. Designing experiments for robust-optimization problems: the Vs-optimality criterion. *IIE Transactions* 2006; **38**(6):445–461.
49. Ye KQ, William L, Sudianto A. Algorithmic construction of optimal symmetric Latin hypercube designs. *Journal of Statistical Planning and Inferences* 2000; **90**:145–159.
50. McKay MD, Beckman RJ, Conover, WJ. A Comparison of three methods for selecting values of input variables in the analysis of output from a computer code. *Technometrics* 1979; **21**(2): 239–245.
51. Iman RL, Helton JC, Campbell JE. An approach to sensitivity analysis of computer models, Part 1. Introduction, input variable selection and preliminary variable assessment. *Journal of Quality Technology* 1981; **13**(3):174–183.
52. Tang B. Orthogonal array-based Latin hypercube. *Journal of the American Statistical Association* 1993; **88**(424); *Theory and Methods*: 1392–1397.
53. Park JS. Optimal Latin-hypercube designs for computer experiments. *Journal of Statistical Planning Inference* 1994; **39**:95–111.
54. Taguchi G, Yokoyama Y, Wu Y. *Taguchi methods: design of experiments*. American Supplier Institute: Allen Park, Michigan, 1993.
55. Owen A. Orthogonal arrays for computer experiments, integration, and visualization. *Statistica Sinica* 1992; **2**:439–452.
56. Seber GAF, Alan JL. *Linear Regression Analysis*. Wiley Interscience: NJ, 2003.

Authors' biographies

Dr. Adel Alaeddini is a Post Doctoral Scholar in the Department of Industrial and Operations Engineering at the University of Michigan-Ann Arbor. His research interests include Statistical Modelling, Global Optimization, and Healthcare Operations Management.

Dr. Alper Murat is an Assistant Professor in the Department of Industrial and Systems Engineering at Wayne State University, Detroit, Michigan. Dr. Murat's research interests include Supply Chain Management, Product Development, Healthcare Systems Engineering, and Data Mining.

Dr. Kai Yang is a Professor in the Department of Industrial and Systems Engineering at Wayne State University, Detroit, Michigan. Dr. Yang's field of expertise includes Quality and Reliability Engineering and Management, Healthcare Systems Engineering, and Product Development.

Dr. Bruce Ankenman is an Associate Professor in the Department of Industrial Engineering & Management Sciences at Northwestern University, Evanston, IL. Dr. Ankenman's field of expertise includes Statistical Design of Industrial and Simulation Experiments, Engineering Design and Development, Quality Improvement and Quality Control, and Applied Statistical Methods.