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Conditionally optimal small composite designs

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Abstract

In this work, we are interested in constructing small composite design for a second-order response surface. A two-stage method is proposed. A proper first-order design with small number of runs would be first selected and then the remaining design points are added, according to an optimal criterion. When the second-order polynomial model is adopted in the second stage, unlike the previous works for small composite designs, not only the proposed method reduces the number of runs for the first-order designs but also decrease the number of adding design points. Here our two-stage method is to find the conditionally optimal small composite designs with only one center point, and a simulated annealing algorithm is used for finding these designs numerically. Based on various types of first-order designs, the corresponding composite designs are found according to D-optimal criterion. These designs are then compared with other small composite designs and minimal-point designs. It is shown that the proposed composite designs perform well in general. In cases where they are not D-optimal, they have reasonably high D-efficiencies. Furthermore, our construction method can be easy extended to the composite designs with more than one center points and to adopt other optimal criteria.

Key words: Central composite design; D-optimality; Point efficiency; Simulated annealing algorithm.

1 Introduction

Response surface methodology (RSM) is connected with fitting a local response surface by a typically small set of observations, and one of the main purposes of RSM is to determine which level combinations of the k input variables (or factors), $x_1, \cdots, x_k$, will optimize the response, y. The challenge of RSM is that the functional relationship between y and $x_1, \cdots, x_k$ is "unknown". Under certain smooth conditions, this response function may be approximated well by lower-order polynomial models over a limited experimental region, $\mathcal{X}$. Usually the first-order polynomial model is employed at the initial stage, i.e.

$$y = \beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k + \varepsilon,$$

where ε is a white noise. If surface curvature exists, then the first-order polynomial model would be modified by adding higher-order terms into the model. Therefore, we might fit a second-order polynomial model of

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{1 \le i < j \le k} \beta_{ij} x_i x_j + \varepsilon,$$

and there are totally $p = \frac{1}{2}(k+1)(k+2)$ parameters in the second-order polynomial model.

One of the popular second-order designs is the central composite design (CCD) introduced by Box and Wilson (1951). There are three portions of a CCD: a 2^k factorial (or fractional factorial with resolution V) design; $2k$ axial points at a distance α from origin, and center points. Here the 2^k factorial (or fractional factorial with resolution V) design and center points are used for fitting the first-order polynomial model and detect the exist of the surface curvature. The $2k$ axial points are then added when the second-order terms are further incorporated. Hence a CCD is extremely useful and powerful in sequential experimentations. However, the total number of the design points (runs) of a CCD is fairly large, especially when k is large. Thus, small composite designs seem more appropriate, especially when experimentation is expensive, difficult, or time-consuming. Searching small composite designs has received a great deal of attention in the literature. Keeping the $2k$ axial points fixed, the first-order designs of CCDs have been replaced by the other small designs, for example: fractional factorial designs with resolution III^* (Hartley, 1959; Draper and Lin, 1990b); irregular fractions of 2^k factorial designs (Westlake, 1965), and Plackett and Burman designs (Draper, 1985, and Draper and Lin, 1990a). From Table 1 in Draper and Lin (1990a), the number of design points of these small composite designs are close to p (the minimal number of design points). For example, with one center point, the small composite designs of Hartley (1959) for $k = 2, 3$ and

6 contain $p+1$ supports. But for the other cases, the number of supports is larger than $p+1$, because of the limitation of the number of runs for the combinatorial designs.

The axial points are added when the second-order polynomial model is employed in the second stage. It is unclear to us why the $2k$ axial points are the only choice. Is it possible to selected fewer added points which still contains "sufficient" information about the true model? In fact, the idea of optimal design could be used to select the added points, since the response model is known at this time. Basically we intend to combine the advantages of both the combinatorial designs and the optimal designs. Thus unlike previous works, our composite designs are constructed in two stages: first choosing a proper combinatorial design to be our first-order design and then adding remaining support points according to an pre-specified optimal criterion over a compact design space.

From optimal design point of view, generally a design ξ is a probability measure over the design space, $\mathcal{X}$. That is the design ξ is represented as

$$\xi = \left\{ \begin{array}{cccc} x_1 & x_2 & \dots & x_n \\ p_1 & p_2 & \dots & p_n \end{array} \right\},$$

where $x_i \in \mathcal{X}$, $i = 1, \cdots, n$, are the distinct support points of ξ, and $p_1, \dots, p_n$ are the weights of ξ that satisfy $\sum_i p_i = 1$ and $p_i \geq 0$. Let $\widehat{\beta}$ be the least-square estimator of the $p \times 1$ parameter vector β of the model. Then the covariance matrix of $\widehat{\beta}$ is

$$Cov(\widehat{\beta}) \propto (M(\xi))^{-1},$$

where $M(\xi) = \int f(x)f'(x)d\xi(x)$ is the information matrix of ξ and $f(x)$ is the $p\times 1$ vector of regressors. By an optimal design, it is to find a design that is "best" with respect to a criterion of the information matrix. For example, a design, ξ^*, is called a D-optimal design if and only if

$$\xi^* = \arg\max_{\xi} |M(\xi)|$$

among all possible designs ξ in $\mathcal{X}$.

Based on our two-stage method, designs considered here can be represented as

$$\xi = \frac{n_c}{n}\xi_c + \frac{n_1}{n}\xi_1 + \frac{n_2}{n}\xi_2, \tag{1}$$

where ξ_c is the one-point design at center point, $\mathbf{0}$, with n_c replications; ξ_1 is the selected first-order design and n_1 is the number of supports of this first-order design; ξ_2 is the equal-weight design for n_2 added points, and $n = n_1 + n_c + n_2$. In particular, ξ can also be written as

$$\xi = \left\{ \begin{array}{cccccccc} \mathbf{0} & x_1 & \ldots & x_{n_1} & a_1 & \ldots & a_{n_2} \\ n_c/n & 1/n & \ldots & 1/n & 1/n & \ldots & 1/n \end{array} \right\}, \tag{2}$$

where $x_1, \ldots, x_{n_1}$ are the distinct supports of the pre-specified first-order design, and $a_1, \ldots, a_{n_2}$ are the unknown added design points. Hence the goal of this work is to find these a_i's according to a particular optimal criterion in a compact design space $\mathcal{X}$. It is clear that the composite design proposed here may not be the optimal design directly derived from the second-order polynomial model, because the all weights and partial design points are fixed. For example, the weight of the center points in the D-optimal designs for the second-order polynomial model with k factors on spherical design spaces, found in Kiefer (1961), is $2/\{(k+1)(k+2)\}$ which may not be equal to n_c/n. In a way, our composite design is treated as a "conditionally" optimal design problem. Namely, given a first-order design with n_c center points, and given a second-order polynomial as the underlying model, what is the optimal design (i.e., optimal design points to be added)? Since our designs are not necessary the optimal design in term the full second-order model, the equivalence theorem in the theory of optimal design can not be used here for identifying these design points. Hence our objective is to directly maximize the objective function derived form the optimal criterion. A simulated annealing algorithm is proposed to find these added supports numerically.

In this work, the composite designs with $p + n_c$ supports are produced, where $p = n_1 + n_2$ and n_c is set to be 1. Thus our small composite design contains $n = p + 1$ supports. This paper is organized as follows. In Section 2, our methodology for constructing the small composite designs with $p + 1$ supports is introduced, and a modified simulated annealing algorithm is proposed for finding added supports. In Section 3, due to the spherical design space and D-optimal criterion, these small composite designs for $k = 2, \cdots, 8$ are found. In Section 4, we compare our proposed designs with other small composite designs and minimal-point designs. Our designs perform well due to the higher D-point efficiencies than these of other small composite designs and minimal-point designs. Finally a conclusion is given in Section 5.

Table 1: The number of supports for the different first-order designs

Factors, k	2	3	4	5	6	7	8
Parameters for second-order polynomials, p	6	10	15	21	28	36	45
2^k full factorial design	4	8	-	-	-	-	-
2^{k-t} resolution V design	-	-	-	16	-	-	-
Plackett and Berman type design	-	4	8	11	16	22	30

2 Proposed methodology

In this section, our two-stage method is introduced. Given a compact design space $\mathcal{X}$ and a optimal criterion, our construction method is in the following:

Stage 1. Choose a proper first-order design and add one center point.

Stage 2. Select the remaining support points according to the optimal criterion over $\mathcal{X}$.

Intuitively, our composite designs combine the advantages of both combinatorial designs and optimal designs: at the first stage of RSM, we use the combinatorial design for factor screening and finding the steepest ascent, and then when the model is known as the second-order polynomial model, the optimal design points are added for the additional experiments. Hence our design problem can be formulated as

$$\xi^* = \arg\max_{\xi_2} \phi(M(\frac{1}{p+1}\xi_c + \frac{n_1}{p+1}\xi_1 + \frac{n_2}{p+1}\xi_2)), \tag{3}$$

where ξ_2 is the equal-weight design of the n_2 added design points, $a_1, \ldots, a_{n_2}$, and $n_2 = p - n_1$. The function, ϕ, is dependent on what criterion we choose. Thus, the goal is to find these unknown added points according to Equation (3).

Here we limit the proper first-order designs to be the 2-level orthogonal designs, and the number of support points of the first-order design is less than p, i.e. $n_1 < p$. The first-order designs that we will consider are shown in Table 1. In CCDs, the distance of axial points from origin is usually set to be $\sqrt{k}$, the square root of the number of factors. Then except the center points, all the other design points (including the first-order design and star portion) are on the surface of the k-ball with radius $\sqrt{k}$, the so-called spherical CCD. Thus, our design space for the case of k factors is set to be the k-ball with radius $\sqrt{k}$.

Since added design points are in k-ball with radius $\sqrt{k}$, these points can be represented in polar coordinate (or spherical coordinate), for example, when $k = 2$, that is

$$(x_1, x_2) = (\sqrt{r}\cos\theta, \sqrt{r}\sin\theta), \tag{4}$$

where θ is the counterclockwise angle from the x_1 axis, and $0 < r \leq k$. Then the function of the information matrix now is also the function of angles and radiuses, and our problem here becomes finding the "best" angles and radiuses, i.e. that maximize (or minimize) a function of the information matrix. As previously mentioned, when the closed form of $\phi(M(\xi))$ can not be derived, we want to search for the added support points numerically.

Since we consider our design problem as an "optimization" problem whose objective function is dependent on what optimal criterion is chosen, then we would like to use a simulated annealing (SA) type algorithm for finding the conditionally optimal composite design designs. The SA algorithm is proposed in Metropolis et al. (1953) and is introduced by Kirkpatrick et al. (1983) as an optimization technique. Since the SA algorithm is a simple procedure for optimization, there are many works applying the SA algorithm to the optimal design problems. For instance, Haines (1987) applied a SA algorithm to construct the exact D-, I- and G-optimal designs for polynomial regression models with uncorrelated errors; Schilling (1992) proposed a SA algorithm for optimal spatial designs with correlated observations, and Angelis et al. (2001) used a SA algorithm to find optimal exact designs in the case of continuous observations with known covariance function. However, these SA algorithms are not suitable for solving our problem here.

First we introduce our SA algorithm. Suppose m is the total number of angles which are to be decided. For simplicity, we use $\theta_1, \cdots, \theta_m$ to index all the angles. Let $\boldsymbol{\theta} = (\theta_1, \cdots, \theta_m)$ and $\boldsymbol{r} = (r_1, \ldots, r_{n_2})$. As mentioned before, the objective function $\phi(\boldsymbol{\theta}, \boldsymbol{r})$ is dependent on the pre-specified criterion. Suppose the objective function, $\phi(\boldsymbol{\theta}, \boldsymbol{r})$, is to be maximized, we define a density

$$\pi_{T(t)}(\boldsymbol{\theta}, \boldsymbol{r}) \propto \exp(\phi(\boldsymbol{\theta}, \boldsymbol{r})/T(t)),$$

where $T(t)$ is the "temperature" at time t and is a decreasing function from initial temperature, $T(0) > 0$, to 0^+. At the t^{th} iteration, the

SA algorithm samples $\boldsymbol{\theta}$ and $\boldsymbol{r}$ from $\pi_{T(t)}(\boldsymbol{\theta}, \boldsymbol{r})$ by a Markov Chain Monte Carlo (MCMC) method. For more information about the SA algorithm, see Chapter 10 of Liu (2001). Here the MCMC method applied for sampling $\boldsymbol{\theta}$ and $\boldsymbol{r}$ is the systematic scan Gibbs sampler. Hence, to maximize $\phi(\boldsymbol{\theta}, \boldsymbol{r})$ with respect to θ_i, $i = 1, \ldots, m$ and r_j, $j = 1, \ldots, n_2$, the **Best Angle and Radius** (BAR) **sampler** is:

1. Select the initial state, $\boldsymbol{\theta}^{(0)}$ and $\boldsymbol{r}^{(0)}$.

2. Run N_t iterations of the Gibbs sampler to sample $\boldsymbol{\theta}$ and $\boldsymbol{r}$ from $\pi_{T(t)}(\boldsymbol{\theta}, \boldsymbol{r})$.

3. Set t to $t + 1$, go to step 1 until t is sufficiently large.

3 Second-order small composite designs for D-optimal criterion

Applying our construction method, the small composite designs with $n = p + 1$ supports for the second-order response surfaces are shown in this section. As mentioned before, there is only one center point in our small composite designs. Therefore, our composite designs are only useful for estimating the parameters for the second-order polynomial directly.

Here D-optimal criterion is used for illustration. The objective function is that

$$\phi(\boldsymbol{\theta}, \boldsymbol{r}) = \phi(\xi) = |M(\xi)| \propto |X(\xi)^{'} X(\xi)|, \tag{5}$$

where $X(\xi)$ is the model matrix of ξ for the second-order polynomial model with respect to $\boldsymbol{\theta}$ and $\boldsymbol{r}$. The value

$$P_{eff}(\xi) = \frac{|X(\xi)^{'} X(\xi)|^{1/p}}{n} \tag{6}$$

is the D-point efficiency (or D-efficiency) of ξ, which is considered as the "information per point" for ξ, and can be used to make the comparisons among designs (see, for example, Qu (2007)).

Due to the properties of the D-optimal criterion, except the center point, we assume all the support points are on the surface of the corresponding design space. Therefore, for each k, our small composite design contains one center point and p design points on the surface of the k-ball with radius $\sqrt{k}$. Hence $r_i = k$, for all $i = 1, \ldots, n_2$, and to find these added points is to search the corresponding best angles. Thus our algorithm can be simplified by sampling angles only, and our objective becomes $d(\boldsymbol{\theta}) = \phi(\boldsymbol{\theta}, \boldsymbol{r}_k)$, where $\boldsymbol{r}_k = (k, \ldots, k)$. Our algorithm is thus called "Best Angle" (BA) sampler.

3.1 Two factors

As seen from Table 1, the first-order design for $k = 2$ is the 2^2 full factorial design. According to the structure of our composite design with only one center point, two added support points are required, because there are 6 parameters in the second-order polynomial model and 4 support points for the 2^2 factorial design. These two added points are represented by polar coordinate, i.e.

$$(x_{11}, x_{12}) = (\sqrt{2}\cos\theta_{11}, \sqrt{2}\sin\theta_{11}) \text{ and } (x_{21}, x_{22}) = (\sqrt{2}\cos\theta_{21}, \sqrt{2}\sin\theta_{21}),$$

where $-\pi \leq \theta_{ij} < \pi$. Thus the determinant of the information matrix of the small composite design is proportional to

$$\begin{aligned} |X(\xi)'X(\xi)| \;=\; & 128[15 + 7\cos(4\theta_{11}) + 7\cos(4\theta_{21}) - 2\cos(\theta_{11} - \theta_{21}) \\ & -2\cos(2(\theta_{11} - \theta_{21})) - 2\cos(3(\theta_{11} - \theta_{21})) - \cos(4(\theta_{11} - \theta_{21})) \\ & -2\cos(2(\theta_{11} + \theta_{21})) - 2\cos(\theta_{11} + 3\theta_{21}) - 2\cos(3\theta_{11} + \theta_{21})]. \end{aligned}$$

In order to find the added D-optimal added points, we take the derivative of $|X(\xi)'X(\xi)|$ with respect to angles, θ_{11} and θ_{21}, and set them to zeros. Using the "solve" function in MATLAB, there are the two candidate classes of angles, θ_{11} and θ_{21}. One class of angles is $(\theta_{11}, \theta_{21}) = \pm(1.4942, 0.0766)$ and $\pm(0.0766, 1.4942)$. Then the two added D-optimal design points are

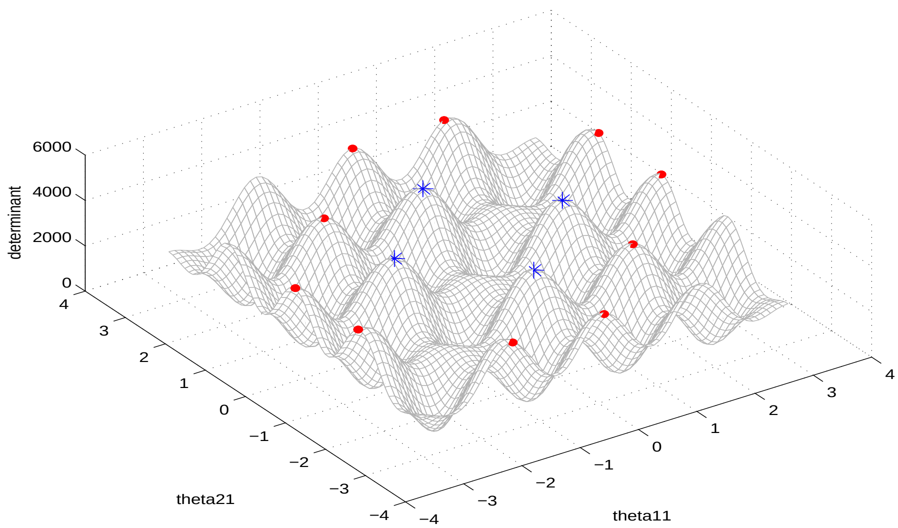
$$\{(1.4101, \pm 0.1082), (0.1082, \pm 1.4101)\} \text{ or } \{(0.1082, \pm 1.4101), (1.4101, \pm 0.1082)\},$$

and the corresponding D-efficiency, $P_{eff} = 0.5733$. The other class of angles is $(\theta_{11}, \theta_{21}) = \pm(-\pi/2, \pi/2)$, $\pm(\pi, 0)$, $\pm(0, \pi)$, $\pm(\pi/2, \pi)$ and $\pm(\pi, \pi/2)$ with D-efficiency, $P_{eff} = 0.5714$. Then the corresponding added points are any two of four axial points,

$$\{\pm(\sqrt{2}, 0), \pm(0, \sqrt{2})\}.$$

Even though this design is not the best design we want, this design still has very high relative efficiency, $0.5714/0.5733 = 0.9968$. The response surface of $|X(\xi)'X(\xi)|$ with respect to θ_{11} and θ_{21} is in Figure

Figure 1: For $k = 2$, the response surface of $|X(\xi)'X(\xi)|$ with respect to θ_{11} and θ_{21}



1. The asterisk points are the angle positions for added D-optimal points, and the circle points are the angle positions for the added supports selected from four axial points.

3.2 Three factors

From Table 1, there are two available first-order designs for $k = 3$, the 2^3 full factorial design and Plackett and Burman design for three factors. Based upon the different first-order designs, the corresponding small composite designs are found as follows.

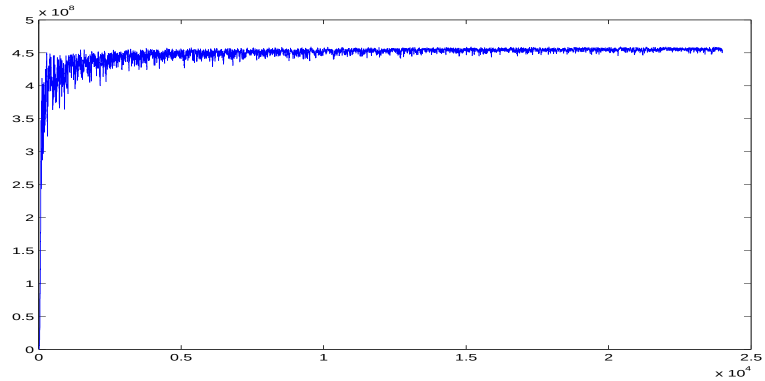
3.2.1 2^3 full factorial design

For $k = 3$, the design space is the 3-ball with radius $\sqrt{3}$. There are 8 design points for the 2^3 factorial design. Thus two added points are required for our small composite design. The spherical coordinates of the two support points are

$$(x_{i1}, x_{i2}, x_{i3}) = (\sqrt{3}\sin\theta_{i2}\cos\theta_{i1}, \sqrt{3}\sin\theta_{i2}\sin\theta_{i1}, \sqrt{3}\cos\theta_{i2}), i = 1, 2,$$

where $0 \leq \theta_{ij} < 2\pi$. Thus the determinant of the information matrix

Figure 2: The determinants of $X(\xi)'X(\xi)$ for $200 \times 10 \times 14 = 28000$ steps when $k = 3$ and the first-order design is the P-B design for three factors



of our small composite design is proportional to

$$\begin{aligned}|X(\xi)'X(\xi)| \quad = \quad & 165888[4\cos 2\theta_{11} - 4\cos 2\theta_{21} - 2\cos(2(\theta_{11} - \theta_{12})) - 6\cos(2(\theta_{21} - \theta_{12})) \\ & -2\cos(2(\theta_{11} + \theta 12)) - 6\cos(2(\theta_{21} + \theta_{12})) + 6\cos(2(\theta_{11} - \theta_{22})) \\ & +2\cos(2(\theta_{21} - \theta_{22})) - 3\cos(2(\theta_{11} - \theta_{12} - \theta_{22})) + 3\cos(2(\theta_{21} - \theta_{12} - \theta_{22})) \\ & -3\cos(2(\theta_{11} + \theta_{12} - \theta_{22})) + 3\cos(2(\theta_{21} + \theta_{12} - \theta_{22})) + 6\cos(2(\theta_{11} + \theta_{22})) \\ & +2\cos(2(\theta_{21} + \theta_{22})) - 3\cos(2(\theta_{11} - \theta_{12} + \theta_{22})) + 3\cos(2(\theta_{21} - \theta_{12} + \theta_{22})) \\ & -3\cos(2(\theta_{11} + \theta_{12} + \theta_{22})) + 3\cos(2(\theta_{21} + \theta_{12} + \theta_{22}))]^2.\end{aligned}$$

We take the derivative of $|X(\xi)'X(\xi)|$ with respect to θ_{11}, θ_{12}, θ_{21} and θ_{22}. Then set these equations to zeros and solve them by the "solve" function in MATLAB. There are twelve solutions of angles. Unlike the case of two factors, the added points are any two perpendicular points selected from 6 axial points, for example: $(\sqrt{3}, 0, 0)$ and $(0, \sqrt{3}, 0)$. The point efficiency of the resulting small composite design is $P_{eff} = 0.6048$.

3.2.2 Plackett and Burman design for three factors

For $k = 3$, another first-order design is formed by columns (1, 2, 3) from the 4-run P-B design. Six added support points are required in this case, and the coordinates of these added points are $x_i = (x_{i1}, x_{i2}, x_{i3}), i = 1, \ldots, 6$. where $x_{i1} = \sqrt{3}\sin\theta_{i2}\cos\theta_{i1}$, $x_{i2} = \sqrt{3}\sin\theta_{i2}\sin\theta_{i1}$, and $x_{i3} = \sqrt{3}\sin\theta_{i2}$. At this time, the close form of the objective function is difficult to write it down. So we find the optimal added points by the BA sampler with $T(t) = (10t)^{-2/3}$ and $N_t = 10$. After 200 iterations, the best point efficiency we get is $P_{eff} = 0.6680$, and the optimal added support points are

$$\begin{pmatrix} 0.2314 & 1.7041 & 0.2058 \\ 1.6997 & 0.2182 & 0.2519 \\ 0.2441 & 0.2502 & 1.6964 \\ -1.0936 & 0.7804 & -1.0931 \\ -1.1209 & -1.0568 & 0.7917 \\ 0.7962 & -1.0902 & -1.0852 \end{pmatrix},$$

where each row is one added design point. From Figure 2, it is clear that an extreme value of $d(\boldsymbol{\theta})$ is found.

3.3 Four and more factors

For $4 \le k \le 8$, the first-order designs are usually formed by P-B designs, except for the case of five factors ($k = 5$), where a 2^{5-1} fractional factorial design is also a candidate design. In all these cases, the closed form of the objective function is hard to derive. Thus, the BA sampler is used here for finding these added design points numerically. As shown before, for BA sampler, we need to set $T(t)$ and N_t first. Currently $T(t)$ is set to be proportional to $t^{-2/3}$ and $N_t = 10$. Here we always check the trend of $|X(\xi)'X(\xi)|$ to see if the number of iterations for the BA sampler is large enough for each case we study, and we still suggest that for each case, we should repeat the BA sampler several times with different initial states to avoid the effect of initial angles for the BA sampler.

For $k = 5$ and 2^{5-1} fractional factorial design as its first-order design, after 400 iterations of our BA sampler, the optimal added design points are

$$\begin{pmatrix} 0.0035 & 2.2353 & 0.0126 & -0.0507 & 0.0292 \\ -0.0166 & 0.0300 & 0.0278 & -2.2327 & 0.1141 \\ 2.2342 & 0.0404 & -0.0109 & -0.0753 & -0.0296 \\ 0.0168 & 0.0220 & 0.0630 & -0.0191 & 2.2349 \\ -0.0156 & 0.0010 & 2.2343 & -0.0699 & 0.0525 \end{pmatrix}$$

with the point efficiency, $P_{eff} = 0.7667$, and these support points are close to five axial points, $(0, \sqrt{5}, 0, 0, 0)$, $(0, 0, 0, -\sqrt{5}, 0)$, $(\sqrt{5}, 0, 0, 0, 0)$, $(0, 0, 0, 0, \sqrt{5})$ and $(0, 0, \sqrt{5}, 0, 0)$. Hence for this case, we believe that

Table 2: The point efficiencies of CCDs and our small composite designs for $k = 2, \cdots, 8$

k	p	$n^{\dagger}_{CCD}$	$P^{\ddagger}_{eff}(CCD)$	$P_{eff}(2^k)$	$P_{eff}(V)$	$P_{eff}(P\text{-}B)$	$\frac{P_{eff}(Small)}{P_{eff}(CCD)}$
2	6	8	0.6285	0.5733	ND	ND	0.9122 2^k
3	10	14	0.7116	0.6048	ND	0.6680	0.8499 2^k 0.9387 *P-B*
4	15	24	0.7673	ND	ND	0.7115	0.9273 *P-B*
5	21	26	0.8002	ND	0.7667	0.7580	0.9581 *V* 0.9473 *P-B*
6	28	44	0.8384	ND	ND	0.7810	0.9313 *P-B*
7	36	78	0.8547	ND	ND	0.6886	0.8057 *P-B*
8	45	80	0.8787	ND	ND	0.6278	0.7145 *P-B*

* ND means "No Design is available".
‡ $P_{eff} = \frac{|X'X|^{1/p}}{n}$, where n is the number of supports of the design.
† n_{CCD} is the numbers of supports of CCDs without center points, while excluding one center point, the number of support points of our small composite design is equal to p.

optimal added points are any five perpendicular axial points from original axial points $(\pm\sqrt{5}, 0, \cdots, 0)$, $\cdots$, and $(0, \cdots, 0, \pm\sqrt{5})$. Thus our composite design is a 2^{5-1} fractional factorial design with resolution V, one center point and five perpendicular points from original ten axial points. For the other cases, the added design points found by our method are shown in Appendix.

When $k \geq 9$, our two-stage method and the BA sampler could also be applied to get the small composite designs. It may take longer computing time to find the added optimal points, however. We would suggest choosing larger N_t and increasing the number of iterations of the BA sampler because the structure of $|X(\xi)'X(\xi)|$ would be more complicated.

4 Comparisons with related work

The point efficiency, Equation (6), can be used to compare designs having different numbers of support points, and the value of P_{eff} is between 0 and 1. The larger P_{eff} value, the better the design is. The P_{eff} values for all our small composite designs are in Table 2. We compare our designs with the spherical CCDs for $k = 2, \cdots, 8$. Here $P_{eff}(CCD)$ is the point efficiency of the spherical central composite design with one center point; $P_{eff}(2^k)$ is the point efficiency of our

Table 3: The relative efficiencies between the small composite designs (SCD) of Hartely (1959), and Draper and Lin (1990a) vs. the proposed small composite designs (Small)

k	Type of design†	$P_{eff}(SCD)$	1st-order design‡	$P_{eff}(Small)$	$\frac{P_{eff}(SCD)}{P_{eff}(Small)}$
2	III^*	0.5714	2^2	0.5733	0.9967
3	III^*	0.5908	2^3	0.6048	0.9769
3	III^*	0.5908	*P-B*	0.6680	0.8844
4	III^*	0.6503	*P-B*	0.7115	0.9140
5	*P-B*	0.5899	V	0.7667	0.7694
5	*P-B*	0.5899	*P-B*	0.7580	0.7782
6	III^*	0.6684	*P-B*	0.7810	0.8558
7	III^*	0.7721	*P-B*	0.6886	1.1213§
7	*P-B*	0.5067	*P-B*	0.6886	0.7358
8	*P-B*	0.4832	*P-B*	0.6278	0.7697

† "Type of design" indicates what small composite design is. The composite designs with resolution III^* designs are proposed by Hartley (1959) and the designs with *P-B* designs are proposed by Draper and Lin (1990a).

‡ the first-order design of our small composite design.

§ In this case, Hartley's design used 10 more support points than the proposed design(47 Vs 37).

small composite design based on the 2^k factorial design; $P_{eff}(V)$ is the point efficiency of our small composite design based on the resolution V design; and $P_{eff}(P\text{-}B)$ is the point efficiency of our small composite design based on the Plackett-Burman design. To compare CCDs with our small composite designs, we use the relative efficiency, i.e.

$$\frac{P_{eff}(Small)}{P_{eff}(CCD)},$$

and the relative efficiencies are shown in the last column of Table 2. It is shown that the relative efficiencies are quite large, except $k = 8$. For the case of $k = 8$ factors, the relative efficiency is 0.7145, but our small composite design require 40% fewer support points than the CCD.

Next, the proposed small composite designs are compared with small composite designs of Hartley (1959) and Draper and Lin (1990a). This is typically done by choosing a good the first-order design of resolution III^* designs and *P-B* designs and then adding the full $2k$

axial points. From Table 3, we see that every $P_{eff}(Small)$ is higher than the corresponding $P_{eff}(SCD)$. Therefore, the proposed small composite designs are superior than these small composite designs. There is an exception, however. For $k = 7$, the point efficiency of Hartley's design with one center point is 0.7721, which is higher than the proposed design, 0.6886. But the number of support points of Hartley's design is 32(first-order) + 14(axial) + 1(center) = 47 which is 10 more support points than our design.

Finally, the proposed small composite designs are compared with other existing minimal-point second-order designs. Here we compare our designs with the designs of Lucas (1974); Notz (1982); Mitchell and Bayne (1976); Box and Draper (1974); Rechtschaffner (1967) and Katsaounis (1999) by point efficiency. The results are shown in Table 4, and the point efficiencies of all these designs were previously published in Katsaounis (1999). From Table 4, the proposed small composite designs are better than the other minimal-point designs, judged by the higher point efficiencies. The proposed designs are better than those minimal-point designs may be due to the following reasons: first, our design is constructed directly to maximize the determinant of the information matrix; secondly, for each k, our design space (spheres) is bigger than the spaces of these minimal-point designs (hypercubes).

Table 4: The comparisons of P_{eff} for selected minimal-point designs

k	Lucas (1974)	Notz (1982)	Mitchell and Bayne (1976)	Box and Draper (1974
3	0.152 (0.251,0.228)	0.400 (0.661,0.599)	0.410 (0.678,0.614)	0.423 (0.699,0.633)
4	0.096 (0.135)	0.392 (0.551)	0.425 (0.597)	0.423 (0.594)
5	0.066 (0.086,0.087)	0.459 (0.598,0.606)	0.456 (0.595,0.602)	0.374 (0.488,0.493)
6	0.048 (0.061)	0.446 (0.571)	ND	0.317 (0.406)
7	0.036 (0.052)	ND	ND	0.227 (0.329)
8	0.028 (0.045)	ND	ND	0.193 (0.307)

Parentheses indicate the relative efficiencies

k	Rechtschaffine (1967)	Katsaounis (1999)		D-optimal Composite design
		V	III^*	
3	0.400 (0.661,0.599)	0.400 (0.661,0.599)	0.410 (0.678,0.614)	0.605 V 0.668 P-B
4	0.392 (0.551)	0.393 (0.552)	0.425 (0.597)	0.712 III^*
5	0.450 (0.587,0.594)	0.459 (0.598,0.606)	0.459 (0.598,0.606)	0.767 V 0.758 P-B
6	0.428 (0.548)	0.446 (0.571)	0.460 (0.589)	0.781 III^*
7	0.383 (0.556)	0.448 (0.650)	0.451 (0.655)	0.689 P-B
8	0.336 (0.535)	0.434 (0.691)	0.446 (0.710)	0.628 P-B

Parentheses indicate the relative efficiencies

5 Conclusion and discussion

A two-stage method for constructing the small composite designs for second-order polynomial models is proposed. When we only have few information about the response surface, a combinatorial design with one center point is chosen for fitting the first-order polynomial model, and then when the second-order polynomial is employed, the remaining supports are selected by a pre-specified optimal criterion. The conditionally optimal designs for $k = 2, \ldots, 8$ are given in details when D-optimal criterion is chosen here. Due to spherical design spaces, the polar coordinate and spherical coordinate are used here to represent the experimental points. When $|X(\xi)'X(\xi)|$ is very complex, we introduce the Best Angle and Radius sampler to find the optimal added points numerically over spherical design spaces, and the results are presented. Other algorithms (such as exchange algorithm in Fedorov (1972) or the procedure OPTEX in SAS) can be applied here too. Since the SA type algorithm can not be guaranteed to find the global extremes of $d(\boldsymbol{\theta})$, (but the local extreme values), we do not claim our composite designs are the global "D-optimal" designs. However, from Tables 2 to 4, the performances of our small composite designs are quite well because the point efficiencies of our designs are larger than those of other small composite designs and minimal-point designs.

In this work, the first-order designs are chosen from the 2-level factorial designs; resolution V designs and P-B designs. When factorial designs ($k = 2, 3$) and resolution V design ($k = 5$) are our first-order designs, added design points usually can chosen from $2k$ axial points. However, when P-B designs are employed as the first-order designs, from our numerical results, axial points should not be the proper choice in terms of D-optimal criterion, but our added design points also contain too many levels. Therefore, to round off levels of our added points should be a way to do. For example, when $k = 3$ and the P-B design is the first-order design, our numerical added points can be rounded as

$$\begin{pmatrix} 0.2500 & 1.6956 & 0.2500 \\ 1.6956 & 0.2500 & 0.2500 \\ 0.2500 & 0.2500 & 1.6956 \\ -1.0000 & 1.0000 & -1.0000 \\ -1.0000 & -1.0000 & 1.0000 \\ 1.0000 & -1.0000 & -1.0000 \end{pmatrix}$$

with the point efficiency, $P_{eff} = 0.7667$. Besides 2-level designs, other combinatorial designs also can be used as our first-order design, because the only one criterion for choosing the first-order design is that $n_1 < p$.

D-optimal criterion is used here for illustrating our method. In fact, any optimal criterion could be employed in stead of D-optimal criterion, for example, ϕ_p-optimal criteria in (Pukelsheim, 1993) or D_s-optimal criterion. Finally our construction method is easy to extend to search the added design points for the composite designs with more than one center point. The case of two factor is demonstrated here. Given the 2^2 full factorial design as the first order design, the two D-optimal added points are found numerically by the BA algorithm for $n_c = 2, 3, 4$. From our numerical results, no matter what n_c is, the D-optimal added points are $(1.4101, 0.1082)$ and $(0.1082, 1.4101)$ (the same as the result of $n_c = 1$), and the corresponding D-point efficiencies are 0.5628, 0.5355 and 0.5056 for $n_c = 2, 3$ and 4 respectively.

Authors' Notes. Dr. Aloke Dey is a true scholar and has been a clear leader in our profession. His work in design of experiment, notably his book co-authored with Mukerjee, has a significant impact in our work. It is our privilege to contribute this work to this special issue in honor of his retirement.

References

Angelis, L., Bora-Senta, E., and Moyssiadis, C. (2001). Optimal exact experimental designs with correlated errors through a simulated annealing algorithm. *Computational Statistics & Data Analysis* **37**, 275-296.

Box, G. E. P. and Wilson, K. B. (1951). On the experimental attainment of optimum conditions. *Journal of the Royal Statistical Society* Ser. B **13**, 1-45.

Box, M. J. and Draper, N. R. (1974). On minimal point second-order designs. *Technometrics* **16**, 613-616.

Draper, N. R. (1985). Small composite designs. *Technometrics* **27**, 173-180.

Draper, N. R. and Lin, D. K. J. (1990a). Small response-surface designs. *Technometrics* **32**, 187-194.

Draper, N. R. and Lin, D. K. J. (1990b). Connections between two-level designs of resolution III^* and V. *Technometrics* **32**, 283-288.

Federov, V. V. (1972). *Theory of optimal experiments*. Translated by Studden, W. J. and Klimko, E. M., Academic press, New York.

Haines, L. M. (1987). The application of the annealing algorithm to the construction of exact optimal designs for linear-regression models. *Technometrics* **29**, 439-447.

Hartley, H. O. (1959). Smallest composite designs for quadratic response surfaces. *Biometrics* **15**, 611-624.

Katsaounis, T. I. (1999). Optimal small response surface designs. *Computing Science and Statistics. Models, Prediction, and Computing. Proceedings of the 31st Symposium on the Interface* **31**, 408-412.

Kiefer, J. (1961). Optimal experimental designs V, with applications to systematic and rotatable designs. *Proc. 4th Berkeley Sympos. Math. Statist. and Probability*, Univ. Calif. Press, Calif., 381-405.

Kirkpatrick, S., Gelatt Jr. C. D. and Vechhi, M. P. (1983). Optimization by Simulated annealing. *Science* **220**, 671-680.

Liu, J. S. (2001). *Monte Carlo Strategies in Scientific Computing.* Springer-Verlag. New York.

Lucas, L. M. (1974). Optimum composite designs. *Technometrics* **16**, 561-567.

Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N. and Teller, A. H. (1953). Equation of state calculation by fast computing machines. *J. Chem. Phys.* **21**, 1087-1092.

Mitchell, T. J. and Bayne, C. K. (1976). D-optimal fractions of three level factorial designs. *Technometrics* **20**, 369-80.

Notz, W. (1982). Minimal point second order designs. *Journal of Statistical Planning and Inference* **6**, 47-58.

Pukelsheim, F. (1993). *Optimal Design of Experiments.* Wiley. New York.

Qu, X. (2007). Statistical Properties of Rechtschaffner Designs. *Journal of Statistical Planning and Inference* **137**, 2156-2164.

Rechtschaffner, R. L. (1967). Saturated fractions of 2^n and 3^n fractional designs. *Technometrics* **9**, 569-575.

Schilling, M. F. (1992). Spatial designs when the observations are correlated. *Commun. Statist.-Simulation* **21**, 243-267.

Westlake, W. J. (1965). Composite designs basd on irregular fractions of factorials. *Biometrics* **21**, 324-336.

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A Appendix

$k = 4$**:** The first-order design is formed by columns (1,2,3,6) from the 8-run P-B design. The coordinates of 7 added points are

$$\begin{pmatrix} 0.2889 & -1.9586 & 0.2831 & -0.0206 \\ 1.9639 & -0.2494 & 0.2817 & 0.0412 \\ -1.2623 & 1.2410 & 0.9262 & 0.0920 \\ 0.9158 & 1.2631 & -1.2504 & 0.0481 \\ -1.1981 & -0.9541 & -1.2845 & 0.0658 \\ -0.0030 & 0.0009 & 0.0322 & 1.9997 \\ 0.2856 & -0.2836 & 1.9579 & 0.0687 \end{pmatrix},$$

and the corresponding point efficiency is $P_{eff} = 0.7115$.

$k = 5$**:** The first-order design is to choose columns (1, 2, 3, 5, 8) from the 12-run P-B design without Run 11. Therefore, there are 11 support points in the first-order design, and 10 added support points are need to be found. After 200 iteration of BA sampler, the best point efficiency we have is 0.7580, and the optimal added support points are

$$\begin{pmatrix} -0.9568 & 1.1070 & -0.9502 & -0.9480 & -1.0282 \\ 2.1733 & 0.2335 & 0.2856 & 0.2635 & 0.2672 \\ 0.2500 & 2.1765 & 0.2578 & 0.2556 & 0.2616 \\ 1.1741 & -0.9144 & -1.0339 & -0.9394 & -0.9132 \\ -0.9399 & -0.9814 & 1.1618 & -0.9492 & -0.9501 \\ -0.8767 & -0.9506 & -1.0020 & 1.1415 & -1.0103 \\ -1.0142 & -0.9468 & -0.9340 & -0.9756 & 1.1184 \\ 0.2171 & 0.2339 & 2.1760 & 0.3156 & 0.2519 \\ 0.2234 & 0.2465 & 0.2391 & 2.1885 & 0.2068 \\ 0.1634 & 0.2391 & 0.2239 & 0.2233 & 2.1946 \end{pmatrix}.$$

$k = 6$: The first-order design is formed by columns (1,2,3,4,5,14) from the 16-run P-B design. After 200 iterations, the best point efficiency is $P_{eff} = 0.7810$, and the optimal added points are

$$\begin{pmatrix}
-2.3790 & 0.4152 & 0.3995 & -0.0425 & 0.0417 & 0.0705 \\
0.0003 & 0.0050 & 0.0193 & 1.4715 & -1.4813 & 1.2805 \\
-1.1891 & -1.5103 & -1.5154 & -0.0287 & 0.0134 & 0.0876 \\
-0.3940 & 2.3887 & 0.3697 & -0.0204 & 0.0373 & 0.0168 \\
1.4935 & -1.4573 & 1.2755 & -0.0949 & 0.0841 & -0.0517 \\
1.4429 & 1.2447 & -1.5390 & 0.0152 & 0.0068 & 0.0152 \\
-0.0410 & 0.0002 & 0.0041 & -2.3972 & 0.3292 & 0.3784 \\
-0.0648 & -0.0189 & -0.0207 & -0.3473 & 2.3971 & 0.3582 \\
0.0241 & 0.0054 & -0.0026 & 1.4462 & 1.2828 & -1.5042 \\
-0.3619 & 0.3687 & 2.3942 & -0.0265 & 0.0004 & 0.0004 \\
-0.0873 & 0.1007 & -0.0151 & -1.2489 & -1.4741 & -1.4997 \\
-0.0132 & 0.0389 & 0.0194 & -0.3793 & 0.3358 & 2.3961
\end{pmatrix}.$$

$k = 7$: For $k = 7$, the first-order design is formed by columns (1, 2, 5, 6, 7, 9, 10) from the 24-run P-B design without Run 3 and Run 20. After 600 iterations, the best point efficiency we have is $P_{eff} = 0.6886$, and the optimal added points are

$$\begin{pmatrix}
-0.6139 & 0.7851 & 0.2010 & -1.4406 & 0.5812 & -1.6563 & 0.8999 \\
-0.1813 & 0.2884 & -0.1198 & 2.5734 & 0.2302 & 0.3296 & 0.2929 \\
0.0902 & -0.4367 & -1.3680 & 0.7627 & -1.1665 & -0.8486 & 1.5057 \\
-0.1654 & 0.1182 & 2.6158 & -0.1737 & 0.2195 & -0.0656 & 0.1830 \\
-2.6174 & 0.1694 & 0.2086 & -0.0754 & 0.1872 & 0.1899 & -0.0169 \\
-0.3954 & -0.1009 & 0.4915 & -0.0443 & 0.4029 & 0.3982 & 2.5038 \\
-0.9594 & -0.8425 & 0.7928 & -0.1242 & 0.4542 & -1.3133 & -1.6717 \\
-0.9151 & -1.0610 & -0.2106 & 0.8952 & -1.7295 & 0.8000 & -0.7485 \\
-0.0259 & 0.3267 & 0.6102 & 0.3332 & 2.5233 & 0.0060 & -0.2054 \\
1.4173 & -0.6425 & 0.2473 & -0.6337 & 0.0765 & 1.0156 & -1.7545 \\
-0.5012 & 0.0222 & 0.1394 & 0.1705 & 0.1735 & 2.5538 & 0.3842 \\
1.0812 & 1.0560 & 0.1219 & -0.9257 & -1.8720 & -0.5169 & -0.2692 \\
-0.1783 & -1.7750 & 0.8848 & -1.4211 & 0.9667 & 0.2786 & -0.0558 \\
-0.2135 & 2.5984 & 0.2424 & 0.1359 & 0.2760 & 0.2153 & -0.0558
\end{pmatrix}.$$

$k = 8$**:** The first-order design is formed by columns (1, 3, 4, 6, 8, 10, 16, 17) from the 36-run *P-B* design without 6 repeat runs, and it contains 30 supports (see Draper and Lin, 1990a). After 600 iterations of our BA sampler, the best point efficiency we get is $P_{eff} = 0.6278$, and the optimal added support points found by the BA sampler are

$$\begin{pmatrix}
0.4529 & 0.1818 & 0.0428 & 2.7018 & 0.0229 & -0.4102 & 0.4058 & 0.3560 \\
0.8844 & 0.3129 & -0.1311 & -0.1769 & 2.6225 & 0.3264 & -0.2952 & 0.0167 \\
-0.7646 & -0.9677 & -1.6676 & 1.2720 & -1.3713 & 0.2750 & -0.1752 & 0.3056 \\
0.3224 & -0.1543 & -0.0468 & 0.3437 & -0.0341 & -2.7440 & 0.3402 & 0.3249 \\
1.0090 & -0.1643 & -0.0284 & 1.1301 & 0.1559 & -0.7308 & -1.8454 & -1.3088 \\
0.5852 & 0.0633 & 2.2280 & 0.2740 & 0.3268 & 1.1059 & -0.9189 & 0.6637 \\
0.2753 & 0.0924 & -0.1168 & 0.2357 & -0.0243 & -0.3760 & 2.7649 & 0.2445 \\
1.0021 & 0.3363 & -0.1116 & 0.8878 & 0.1645 & 1.8034 & 0.7905 & -1.4758 \\
0.6249 & 0.5341 & -2.5706 & 0.0130 & 0.5149 & -0.0591 & -0.5878 & 0.3193 \\
-1.7917 & -0.2162 & 0.0631 & 1.1246 & -0.2783 & -1.0204 & 1.0522 & -1.1173 \\
-1.0074 & -0.0302 & 0.0404 & -1.4944 & 0.0079 & 1.3561 & -1.2892 & 1.1173 \\
2.7788 & 0.0001 & -0.0040 & 0.2951 & 0.2162 & -0.2337 & 0.2251 & 0.1980 \\
0.4574 & 2.6645 & -0.3403 & 0.1879 & 0.4196 & 0.5598 & 0.1305 & 0.1831 \\
1.0901 & -0.1960 & 0.0269 & -2.0193 & 0.2239 & -0.7220 & 0.9578 & -1.0982 \\
0.2375 & 0.0086 & -0.1047 & 0.2319 & 0.0261 & -0.3652 & 0.4717 & 2.7427
\end{pmatrix}.$$