

A NOTE ON CONDITIONALLY OPTIMAL STAR POINTS IN CENTRAL COMPOSITE DESIGNS FOR RESPONSE SURFACE METHODOLOGY

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ABSTRACT

In this paper, conditionally optimal star points in central composite designs for second-order response are considered. The central composite design consists of three portions: factorial, center and star points. Suppose that factorial design and certain center points have been conducted, we seek the optimal $2k$ star points in the sense of A -optimality. When k is large, a simulated annealing algorithm is used to search the corresponding A -optimal star points. It is shown that A -optimal star points remain on the axes, but the distance to the origin depends on the number of center points. These are very different from the classical central composite designs. Optimal star points for other optimality criteria are also discussed.

Key words and phrases: A -optimality, A_s -optimality, conditionally optimal design, D -optimality, simulated annealing.

JEL classification: C61, C99.

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1. Introduction

The central composite design (CCD), proposed by Box and Wilson (1951), is probably the most popular second-order designs. It is very efficient for the sequential experiments especially in response surface methodology (RSM). In the first stage of response surface methodology, a 2^k factorial design (or resolution V design for large k) and certain center points are used for fitting the first-order polynomial model of k factor, i.e.

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

where y is the response variable, x_1, \dots, x_k are the k factors, β_0, \dots, β_k are the unknown parameters, and ε is a random variable with mean 0 and variance σ^2 . When surface curvature does exist, the second-order terms are incorporated to the first-order polynomial model into a second-order polynomial model, i.e.

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

where β_{ij} are the unknown parameters for the quadratic and interaction terms. The $2k$ star points would be added to form the composite design. These star points are fixed on the axes and can be represented as $(\pm\alpha, 0, \dots, 0), \dots, (0, \dots, 0, \pm\alpha)$, where α is the distance from the origin.

Two important parameters in central composite design need to be specified, the number of center points (n_c) and the star distance (α). To select n_c , Box and Draper (1963) used a variance-plus-bias criterion; Lucas (1977) applied the criteria of D -efficiency and G -efficiency; Draper (1982) proposed the integrated variance criterion, and Lim and So (2001) used c -efficiency. For suitable value of α , it can be determined by the rotability property. In Myers and Montgomery (1995) the variance dispersion graphs were used to compare central composite designs with different α 's. In all of these studies, all of the star points are fixed on the axes. However, it is not clear why these $2k$ star points must be on axis. The goal of this paper is to simultaneously study both the effect of n_c and the "best" location of the star points (including the value of α) following the two-stage procedure in response surface methodology.

We employ an optimal design approach in achieving this goal. Given a first-order design with n_c center points, we are interested in how to select the additional experimental points (star points). This approach is intuitively sensible especially for response surface methodology. In the first stage of response surface methodology, little prior information about the true surface is known. Thus the first-order polynomial model would appear to be a proper choice, and consequentially a fractional factorial design is used. If the curvature of the response surface does exist, then a second-order polynomial model is appropriate for fitting the curvature of the true response surface and additional experimental points are needed. To obtain a better estimation of the parameters

in this new second-order polynomial model, we design these additional experimental points based upon a design optimality criterion conditionally on the first-order design. We therefore treat our designs as “conditionally optimal designs”. Chen et al. (2008) used a similar idea to obtain small composite designs based on D -optimality.

In optimal designs, a design ξ is generally a probability measure over the pre-specified design space, \mathcal{X} . Given this, the central composite designs considered here can be represented as

$$\xi = \left\{ \begin{array}{cccccc} \mathbf{0} & x_1 & \dots & x_{n_1} & s_1 & \dots & s_{2k} \\ n_c/n & 1/n & \dots & 1/n & 1/n & \dots & 1/n \end{array} \right\}, \quad (1)$$

where $\mathbf{0} = (0, \dots, 0)$ is the center point, x_1, \dots, x_{n_1} are the supports (or design points) of the first-order design (2^k factorial design or resolution V design for large k), and s_1, \dots, s_{2k} are the additional star points. Thus here the total number of runs (design points), n , is equal to $n_c + n_1 + 2k$. Let $\hat{\beta}$ be the least-square estimator of the parameter vector β of the second-order polynomial model with uncorrelated error. The covariance matrix of $\hat{\beta}$ is then proportional to the information matrix of ξ , $M(\xi) = X'X/n$, i.e.

$$Cov(\hat{\beta}) \propto \left(\frac{1}{n}X'X\right)^{-1} = M^{-1}(\xi),$$

where X is the model matrix corresponding to the design ξ . In fact, to find a optimal design is to optimize this covariance matrix in some senses. Here the A -criterion is considered (other criteria will be discussed later).

An A -optimal design, ξ_A^* , which minimizes the sum of the variances of regression parameters, is defined as:

$$\xi_A^* = \arg \min_{\xi} \text{trace}M^{-1}(\xi) = \arg \min_{\xi} \text{trace}(X'X)^{-1}.$$

This A -optimal criterion is particularly important for the situation when the confidence ellipsoid of the parameter estimations is appears as long and thin because such a case would result in comparatively poor estimation of one or more parameters. Müller (1994) also showed that A -optimal designs are optimal for the optimal robust estimation in linear models whose error terms may have differently contaminated normal distributions. For more details about A -optimal designs, please see Atkinson and Donev (1992), and Pukelsheim (1993). To compare two designs under the A -optimal criterion, the measure of the relative A -efficiency of ξ_1 and ξ_2 is given by:

$$\text{trace} M^{-1}(\xi_2)/\text{trace}M^{-1}(\xi_1) = \text{trace}(X_2'X_2)^{-1}/\text{trace}(X_1'X_1)^{-1}, \quad (2)$$

where X_1 and X_2 are the model matrices for ξ_1 and ξ_2 , respectively.

The goal of our work here is to identify s_1, \dots, s_{2k} from the pre-specified design space, \mathcal{X} , according to the A -optimal criterion. It is clear that our composite designs are not necessarily the optimal designs for the full second-order polynomial model as

the weights of our composite designs are fixed, and parts of our composite designs are combined with fractional factorial designs and center point. For example, the D -optimal design for the second-order polynomial model of k factors on a k -ball was found in Kiefer (1961), and in this D -optimal design, the weight for the center point is $2/(k+1)(k+2)$, which might not be equal to n_c/n . Thus the equivalence theorem in optimal design cannot be directly applied to enable us to identify the optimal additional points, s_i 's. The optimal additional points are therefore obtained via a direct optimization of an objective function, which is the trace of the inverse of the information matrix. A simulated annealing algorithm is proposed to find designs numerically. This is particularly useful when the objective function is too complex.

This paper is organized as follows. In Section 2, our methodology for selecting the optimal $2k$ star points from the design space is introduced, and a modified simulated annealing algorithm is proposed for finding additional design points. The optimal $2k$ additional design points for $k = 2, \dots, 8$ are given in Section 3, followed by a thorough comparison with spherical central composite designs by relative A -efficiencies. Finally a conclusion and a discussion of other criteria are given in Section 4.

2. Selection Method

Spherical central composite designs for k factors, that set $\alpha = \sqrt{k}$, are commonly used in practice, because all of the other experimental points are on the boundary of the ball with radius \sqrt{k} except for the center points. Thus such a design space, \mathcal{X} , is used here. Specifically, our goal is to find the $2k$ star points, s_1, \dots, s_{2k} , according to the A -optimal criterion for the k -ball with radius \sqrt{k} .

Due to spherical design space, it is convenient to represent these additional points by polar coordinates or spherical coordinates. For example, when $k = 2$, this is

$$(x_1, x_2) = (r \cos \theta, r \sin \theta),$$

where $r = \sqrt{x_1^2 + x_2^2}$ is the radial distance from the origin, and θ is the counterclockwise angle from the x_1 axis. Following the same structure of the central composite design, it is desirable that these additional $2k$ star points satisfy symmetric and orthogonal properties. We therefore add $2k$ symmetric design points from each quadrant of the k -sphere with radius r "uniformly". The additional points in each half-space, $\{\mathbf{x} = (x_1, \dots, x_k) | x_i \geq 0\}$, $i = 1, \dots, k$ are perpendicular to each other. For $k = 2$, these four additional points, s_1, \dots, s_4 , are denoted by:

$$(r \cos \theta, r \sin \theta), (-r \sin \theta, r \cos \theta), (r \sin \theta, -r \cos \theta), \text{ and } (-r \cos \theta, -r \sin \theta),$$

where $0 < r \leq \sqrt{2}$, and $0 \leq \theta < \frac{\pi}{2}$. In fact, the four additional points for $k = 2$ can also be considered to rotate axial points, whose distances from origin are r , by an angle θ .

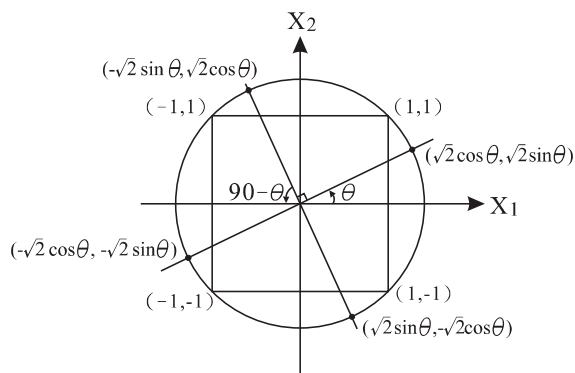


Figure 1: The positions of four additional points when $k = 2$ and $r = \sqrt{2}$.

Since two orthogonal vectors rotated through an angle θ can be performed by multiplication with a Givens rotation matrix, the coordinates of these four additional points can also be written as:

$$G_{12}(\theta) \begin{pmatrix} r & 0 \\ 0 & r \end{pmatrix} \text{ and } -G_{12}(\theta) \begin{pmatrix} r & 0 \\ 0 & r \end{pmatrix} \tag{3}$$

where $G_{12}(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$ is a 2×2 Givens rotation matrix for axes x_1 and

x_2 , and angle θ . Hence generally, the $2k$ additional points, s_1, \dots, s_{2k} , are represented as:

$$\pm \prod_{i < j} G_{ij}(\theta_{ij}) D_k(r) \tag{4}$$

where $D_k(b)$ is a $k \times k$ diagonal matrix with the diagonal element, b , and $G_{ij}(\theta_{ij})$ is a k -dimensional Givens rotation matrix which is representing a rotation in the plan spanned by the i^{th} and the j^{th} axes ($i < j$) through an θ_{ij} . Figure 1 is an illustration of our approach for the case of two factors.

For the A -optimal criterion, the optimal $2k$ additional points are found such that the corresponding trace of the inverse of the information matrix is minimized. Since all $2k$ additional points are represented by (4), the objective function, $trace M^{-1}(\xi)$, is a function of r and θ_{ij} , i.e.

$$trace M^{-1}(\xi) = d_A(r, \theta_{12}, \dots, \theta_{(k-1)k}).$$

Therefore, to find the $2k$ optimal additional points, we minimize the objective function directly with respect to r and θ_{ij} . The formulation of our objective function would be complicated for large k , because of the complexity of the information matrix. In such a case we search for the optimal additional points numerically.

In optimal design problems, an exchange algorithm, such as SAS's procedure OP-TEX, can be used for searching the additional design points according to some criteria. However, here the additional points must satisfy the orthogonal property and such exchange algorithms cannot be applied directly. Since the simulated annealing algorithm is simple, powerful, and has been widely used in optimal design problems (see, for instance, Fang and Wiens, 2000), we will modify the simulated annealing for our specified needs.

To minimize the objective function $d(r, \theta_1, \dots, \theta_p)$, define a density

$$\pi_{T(t)}(r, \theta) \propto \exp(-d(r, \theta)/T(t)),$$

where $\theta = (\theta_1, \dots, \theta_p)$, and $T(t)$ is the "temperature" at time t and is a function decreasing from the initial temperature, $T(0) > 0$, to 0^+ . Following the algorithm in Liu (2001), our MCMC version simulated annealing algorithm is as follows:

1. Select the initial angles, $\theta_i^{(0)}$, $i = 1, \dots, p$, and initial radius, r^0 , $0 < r^0 \leq \sqrt{k}$.
2. Run N_t iterations of the Gibbs sampler to sample r and θ from $\pi_{T(t)}(\theta)$. At each iteration of the Gibbs sampler,
 - (1) Sample r from $\pi_{T(t)}(r|\theta)$ and
 - (2) Draw θ_i , $i = 1, \dots, p$, from $\pi_{T(t)}(\theta_i|r, \theta_{-i})$.
3. Set t to $t + 1$, repeat these steps until t is large enough.

Here θ_{-i} is the set of all angles θ_j except the i^{th} angle, i.e. $\theta_{-i} = (\theta_1, \dots, \theta_{i-1}, \theta_{i+1}, \dots, \theta_p)$. This algorithm is called as the Best Angles and Radius sampler (BAR sampler in short). Since the simulated annealing algorithm may be affected by the initial states, we would repeat the BAR sampler several times with different initial angles and radii selected at random to make sure the optimum values are found. For each replication, we also check the trend of the values of $d(r, \theta)$ at each iteration of the BAR sampler to make sure that $d(r, \theta)$ is really close to an extreme value. Note that, for this BAR sampler, the Metropolis-Hastings algorithm can be used instead of the Gibbs sampler. We believe that the performance would then be similar to what we have found here.

3. A -optimal Star Points

The $2k$ A -optimal additional points for the composite design found are shown in this section. The closed form of the objective function is first attempted. When this is too complicated, the BAR sampler is applied to obtain the results numerically.

3.1 Two ($k = 2$) Factors

When $k = 2$, the four additional points are represented as (3) with radius r and angle θ_{12} . We then show that these four A -optimal additional points are on the axes by a straightforward computation of $\text{trace}(X'X)^{-1}$. Based on the 2^2 factorial design and n_c center points, the trace of the inverse of the information matrix $M(\xi)$ is proportional to

$$d_{A,2,n_c}(r, \theta_{12}) = \text{trace}(X'X)^{-1} = \frac{1}{8} \left(\frac{48(6 + n_c) + 8(10 - n_c)r^2 + 10(4 + n_c)r^4 + (12 + n_c)r^6}{(2 + r^2)(4(2 - r^2)^2 + n_c(4 + r^4))} + \left(1 + \frac{4}{r^4}\right) \sec^2(2\theta_{12}) \right).$$

For any r , the minimum value of $d_{A,2,n_c}(r, \theta_{12})$ is attained when $\theta_{12} = 0$. Thus these four A -optimal star points are all on axes.

Now the A -optimal star points for $k = 2$ are found by minimizing $d_{A,2,n_c}(r, 0)$ with respect to r , $0 < r \leq \sqrt{2}$. Here we consider the cases of $n_c = 1, 2, 3$ and 4.

$n_c = 1$: When $n_c = 1$, to minimize $d_{A,2,1}(r, 0)$, we take the derivative of $d_{A,2,1}$ with respect to r , and set it to zero. Then we use the “NSolve” function in Mathematica to obtain the solution. The minimum of $d_{A,2,1}(r, 0)$ is achieved when $r = 1.0311$. Hence the A -optimal star points are $(1.0311, 0)$, $(-1.0311, 0)$, $(0, 1.0311)$ and $(0, -1.0311)$. Thus, the A -optimal star points are indeed on the axes, but not at $(\pm\sqrt{2}, 0)$ or $(0, \pm\sqrt{2})$ (which are the original star points of spherical CCD for $k = 2$).

$n_c = 2, 3, 4$: When $n_c > 1$, we are only able to show that $d_{A,2,n_c}(r, 0)$ is a monotone decreasing function for $0 < r \leq \sqrt{2}$. Therefore, for $n_c = 2, 3$ and 4, the A -optimal star points are $(\sqrt{2}, 0)$, $(-\sqrt{2}, 0)$, $(0, \sqrt{2})$ and $(0, -\sqrt{2})$, which are the same as the original star points of the spherical CCD.

3.2 More than Two Factors

Here the number of factors is more than two. The $2k$ symmetric design points are represented by (4). For simplicity, we use $\theta_1, \dots, \theta_p$ ($p = (k - 1)k/2$) to index all of the angles. Since the trace of the inverse of the information matrix is quite complicated, the BAR sampler is applied to find the A -optimal star points for k , $3 \leq k \leq 8$. We also set $n_c = 1, 2, 3$ and 4. Our task now is to minimize the trace of the inverse of $X'X$ numerically. The density $\pi_{T(t)}(r, \theta)$ in our BAR sampler is defined as $\pi_{T(t)}(r, \theta) \propto \exp(-d_{A,k,n_c}(r, \theta)/T(t))$, where $d_{A,k,n_c}(r, \theta) = \text{trace}(X'X)^{-1}$. As previously mentioned, BAR sampler is repeated several times with different initial states which are selected randomly to make sure that the minimal value is obtained.

We next show the details for the case of $k = 3$.

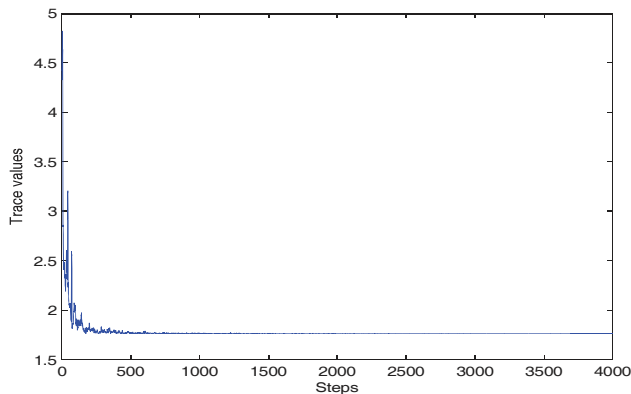


Figure 2: For $k = 3$ and $n_c = 1$, the trace of $(X'X)^{-1}$ of the BAR sampler for 100 iterations ($4 \times 10 \times 100 = 4000$ steps)

When $k = 3$, there are one r , $0 < r \leq \sqrt{3}$ and three angles, θ_1, θ_2 and θ_3 . We iterate the BAR sampler 100 times, and set $N_t = 10$ and $T(t) \propto t^{-2}$.

$n_c = 1$: When $n_c = 1$, the six A -optimal additional points we find are $\pm(1.2557, -0.0017, 0.0007)$, $\pm(0.0017, 1.2557, 0.0001)$ and $\pm(-0.0007, -0.0001, 1.2557)$. These A -optimal additional points are not the original star points in the spherical CCD. However, the additional points are still on axes at a distance 1.2557 from origin. Figure 2 displays the trend of the trace of $(X'X)^{-1}$ of the BAR sampler. From this figure, $d_{A,3,1}(r, \theta)$ converges rapidly to the minimum.

$n_c = 2, 3, 4$: When $n_c = 2, 3$ and 4 , the numerically A -optimal star points are all close to the $2k$ original star points, i.e. $(\pm\sqrt{3}, 0, 0), (0, \pm\sqrt{3}, 0), (0, 0, \pm\sqrt{3})$. For example, taking $n_c = 4$, these six A -optimal star points are $\pm(1.7321, 0.0007, -0.0001)$, $\pm(-0.0007, 1.7321, 0.0001)$ and $\pm(0.0001, -0.0001, 1.7321)$.

Thus the A -optimal star points remain on axes, but the distance to the origin depends on the number of center points, n_c . These results are coincident with the case of $k = 2$.

The BAR sampler is also used for finding the $2k$ A -optimal star points numerically for the other cases, $k = 4, \dots, 8$. For $k = 4, \dots, 8$, the A -optimal additional points are on axes, but the distance from these points to the origin varies with n_c . Table displays the optimal radii found by the BAR sampler (r) and compares with \sqrt{k} by their ratio r/\sqrt{k} . From this table, we see that the more center points, the larger the distance from origin is and the distance is usually less than \sqrt{k} with small n_c . For example, when $k = 8$, the best r for $n_c = 1, 2, 3$, and 4 are all less than $\sqrt{8} = 2.2824$, and the optimal r is close to $\sqrt{8}$ when n_c is getting larger. When the distance is equal to \sqrt{k} , the original star points, $(\pm\sqrt{k}, 0, \dots, 0), \dots, (0, \dots, 0, \pm\sqrt{k})$, in the spherical central composite designs are also the A -optimal additional points.

Table 1: The best radiuses of A -optimal central composite designs.

Factors (k)	$n_c = 1$	$n_c = 2$	$n_c = 3$	$n_c = 4$
2	1.0311 (0.7291)	1.4142 (1.0000)	1.4142 (1.0000)	1.4142 (1.0000)
3	1.2557 (0.7250)	1.7321 (1.0000)	1.7321 (1.0000)	1.7321 (1.0000)
4	1.4420 (0.7210)	1.5980 (0.7990)	2.0000 (1.0000)	2.0000 (1.0000)
5	1.6040 (0.7173)	1.7426 (0.7793)	2.2361 (1.0000)	2.2361 (1.0000)
6	1.7571 (0.7173)	1.8665 (0.7620)	2.0135 (0.8220)	2.4495 (1.0000)
7	1.8979 (0.7173)	1.9914 (0.7527)	2.1025 (0.7947)	2.6457 (1.0000)
8	2.0233 (0.7153)	2.1119 (0.7467)	2.2137 (0.7827)	2.3438 (0.8287)

Note: Parentheses indicate the ratios of r and \sqrt{k} , i.e. r/\sqrt{k} .

3.3 Comparison with Spherical Central Composite Designs

To compare our conditionally A -optimal central composite designs with spherical central composite designs, we use the relative A -efficiency in (2). The relative A -efficiency of our conditionally A -optimal central composite design and spherical central composite design is defined as:

$$traceM^{-1}(\xi_A)/traceM^{-1}(\xi_{CCD}),$$

where ξ_A is our conditionally A -optimal central composite design and ξ_{CCD} is the spherical central composite design. When this relative efficiency is less than 1, our conditionally A -optimal central composite design is better than the corresponding spherical central composite design. The relative A -efficiencies and the values of the trace of $(X'X)^{-1}$ are displayed in Table 2. From this table we see that our conditionally A -optimal central composite designs have better or same performance than the spherical central composite designs. This is especially true when n_c is small (for instance $n_c = 2$ and $k = 4, \dots, 8$). In such cases our conditionally A -optimal central composite designs are better than the corresponding spherical central composite designs. The relative efficiencies decrease as k increases, except in the case of $k = 8$ and $n_c = 1$. Also note that, for large n_c , both designs have the similar trace values.

Table 2: The relative efficiencies of our conditionally A -optimal central composite designs and the spherical central composite designs. When the relative efficiency is less than 1, our proposed design is better (and thus different) than the central

Factors (k)	$n_c = 1$	$n_c = 2$	$n_c = 3$	$n_c = 4$
2	0.97522 (2.1333)	1.0000 (1.4375)	1.0000 (1.1875)	1.0000 (1.0625)
3	0.8567 (1.7626)	1.0000 (1.3909)	1.0000 (1.1687)	1.0000 (1.0575)
4	0.7556 (1.4324)	0.9921 (1.2607)	1.0000 (1.0625)	1.0000 (0.9583)
5	0.7555 (1.5903)	0.9722 (1.4632)	1.0000 (1.3050)	1.0000 (1.2050)
6	0.6655 (1.2278)	0.9050 (1.1418)	0.9998 (1.0670)	1.0000 (0.9700)
7	0.5795 (0.9410)	0.8342 (0.8779)	0.9553 (0.8234)	1.0000 (0.7666)
8	0.5864 (1.0079)	0.8279 (0.9572)	0.9421 (0.9126)	0.9969 (0.8723)

composite design.

Note: Parentheses indicate trace of $(X'X)^{-1}$ of our conditionally optimal central composite designs.

4. Conclusion and Discussion

In this paper, we are mainly interested in which $2k$ additional design points should be added when the first-order design and center points are given. Following the basic idea of central composite design, the symmetric and orthogonal star points are found over the spherical design space according to an optimal criterion. Since the design space is a k -ball, polar (or spherical) coordinates are used to represent all support points. Because these star points must satisfy the orthogonal property, the Givens rotation matrix is applied to rotate orthogonal vectors here. Thus, our objective functions are functions of rotation angles and radial distance from origin. A simulated annealing algorithm, the Best Angle and Radius sampler, was then used to optimize the objective functions. A -optimal star points were obtained and displayed for $k = 2, \dots, 8$. It can be seen that, with the small number of center points, the A -optimal star points are still on the axes, but may be in the k -ball with radius \sqrt{k} .

When more center points are added, a better estimation of the intercept term is anticipated. To see the effect of the intercept term in the newly constructed designs, conditionally A_s -optimal designs are also studied here. Namely, all parameters except for the intercept term in the second-order polynomial model, i.e. $(\beta_1, \dots, \beta_k, \beta_{11}, \dots, \beta_{kk}, \beta_{12}, \dots, \beta_{(k-1)k})$ are investigated. See Chapter 10.6 of Atkinson and Donev (1992) for details. It is shown that the original star points are the A_s -optimal star points. This provides a good reason for why our A -optimal star points are closer to the origin than \sqrt{k} when fewer center points are chosen.

Generally the optimal criterion can be represented by the ϕ_p -criterion, $p \in (-\infty, 1]$. The ϕ_p -optimal design seeks to maximize $\phi_p(M(\xi))$, where $M(\xi)$ is a symmetric non-negative definite $h \times h$ matrix, and

$$\phi_p = \begin{cases} (\frac{1}{h} \text{trace} M^p(\xi))^{1/p}, & \text{for } p \neq 0 \\ (\det M(\xi))^{1/h}, & \text{for } p = 0. \end{cases}$$

In fact, the A -criterion is a special case of the ϕ_p -criterion with $p = -1$, and when $p = 1$, the ϕ_1 -criterion is the D -criterion. For more details regarding the ϕ_p -criterion, please see Pukelsheim (1993). Our BAR sampler is easily employed to search the ϕ_p -optimal additional points over the spherical design spaces numerically by setting the density, $\pi_{T(t)}$, to be:

$$\pi_{T(t)}(r, \theta) \propto \exp(\phi_p(\xi)/T(t)). \quad (5)$$

For the D -criterion, (5) becomes $\pi_{T(t)}(r, \theta) \propto \exp(\det(X'X)/T(t))$. For $k = 2, \dots, 8$, the D -optimal star points found by the BAR sampler over the k -ball with radius \sqrt{k} are $(\pm\sqrt{k}, 0, \dots, 0), \dots, (0, \dots, 0, \pm\sqrt{k})$.

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對於反應曲面法的中央合成設計實驗之最佳星點設計研究 隨機效率前緣方法實證研究

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摘要

在此論文中，我們探討在二次反應曲面模型下的中央合成設計之最佳星點設計問題。中央合成設計包含了三個部份：部分因子設計、中心點及星點。在已經執行部分因子設計及中心點的實驗假設下，我們以 A-最適設計準則來尋找最佳星點的位置。另外亦提出一個模擬退火演算法以求其最佳星點的數值解。由數值試驗結果發現一些與傳統中央合成設計相異的特性。因為雖然 A-最佳星點依然落於各個座標軸上，但其與中心點的距離卻與中心點的實驗數有關。最後在此論文中亦有討論將其他的最適設計準則。

關鍵詞：A-最適設計準則, As-最適設計準則, 有條件下之最適設計, D-最適設計準則, 模擬退火演算法。

JEL classification: C61, C99.