A Study on Minimal-point Composite Designs

by

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Contents

1 Introduction 1

2 Construction for Minimal-point Designs 3
   2.1 The restriction for first-order designs  . . . . . . . . . . . . . . . . . . 4
   2.2 The numerical method for finding added support points  . . . . . . . . 5

3 Minimal-point Designs 8
   3.1 \( A \) - and \( A_s \)-optimal minimal-point composite designs  . . . . . . . . 8
      3.1.1 \( A \) - and \( A_s \)-optimal minimal-point composite designs for \( k = 2 \)  . 10
      3.1.2 \( A \) - and \( A_s \)-optimal minimal-point composite designs for \( k = 3 \)  . 12
      3.1.3 \( A \) - and \( A_s \)-optimal minimal-point composite designs for \( k = 4 \)  . 13
      3.1.4 \( A \) - and \( A_s \)-optimal minimal-point composite designs for \( k = 5 \)  . 15
      3.1.5 \( A \) - and \( A_s \)-optimal minimal-point composite designs for \( k = 6 \)  . 18
      3.1.6 \( A \) - and \( A_s \)-optimal minimal-point composite designs for \( k = 7 \)  . 20
   3.2 Slope-rotatable minimal-point composite designs  . . . . . . . . . . . . . . . . . 22
      3.2.1 Slope-rotatable minimal-point composite designs for \( k = 2 \)  . . . 23
      3.2.2 Slope-rotatable minimal-point composite designs for \( k = 3 \)  . . . 25
      3.2.3 Slope-rotatable minimal-point composite designs for \( k = 4 \)  . . . 25
      3.2.4 Slope-rotatable minimal-point composite designs for \( k = 5 \)  . . . 26
      3.2.5 Slope-rotatable minimal-point composite designs for \( k = 6 \)  . . . 28
      3.2.6 Slope-rotatable minimal-point composite designs for \( k = 7 \)  . . . 28

4 Comparisons 29

5 Conclusion 35

A Appendix:
   The Figures of \( A \)- and \( A_s \)-optimal and Slope-rotatable Criteria 36
   A.1 \( A \)-optimal minimal-point composite designs  . . . . . . . . . . . . . . . 37
   A.2 \( A_s \)-optimal minimal-point composite designs  . . . . . . . . . . . . . . . . . 40
A.3 slope-rotatability minimal-point composite designs . . . . . . . . . . . . . . . . . . . . 43

References 45
最少點合成設計的研究

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摘要

在本篇論文裡，我們有興趣的是在二階反應曲面的假設下去建構一個最少點設計。在本論文中使用一個兩階段法去建構這些最少點設計。在一第一個階段，先選定一個有較少實驗點的適當一階模型設計。然後，在第二階段裡，依據不同的準則之下，找出這些剩餘實驗點。在這裡我們除了有A-最佳準則之外，還有A_n-最佳準則及可旋轉的斜率準則。因此，根據不同的準則，基於三種不同型式的一階模型設計，使用模擬退火演算法來尋找這些對應的最少點設計。最後我們利用相對效率來比較我們所找到的最少點設計和其他的小型合成設計及最少點設計。一般而言，我們提出的合成設計有不錯的結果。

關鍵字：中央合成設計、A-最佳準則、A_n-最佳準則、可旋轉的斜率準則、模擬退火演算法
A Study on Minimal-point Composite Designs

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ABSTRACT

In this work, we are interested in constructing minimal-point designs for second-order response surface. A two-stage method is used for finding the composite designs. First we choose a proper first-order design with small supports, and then the remaining supports are selected according to an pre-specified criterion. A modified simulated annealing algorithm is applied here for numerically finding these added supports according to the different criteria. Besides $A$-optimal criterion, $A_s$-optimal and slope-rotatable criteria are also used here. Based on the three different types of first-order designs, the corresponding minimal-point designs are found. Finally these designs are compared with central composite designs, other small composite designs and minimal-point designs by relative efficiencies. It is shown that the proposed composite designs perform well in general.

Keywords: Central composite designs, $A$-optimal criterion, $A_s$-optimal criterion, slope-rotatable criterion, 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 the purpose of RSM is to determine what levels of the independent variables maximize or minimize the response. In RSM, the challenge is that the functional relationship, \( f \), between the response \( y \) and the independent variables (factors), \( x_i, \ i = 1, 2, \ldots, k \), is “unknown”. Under certain smooth assumptions, this function, \( f \), shall be approximated well by lower-order polynomial models over a limited experimental region, \( \mathcal{X} \). There are two polynomial models used in RSM. The first approximation model is the first-order polynomial model, i.e.

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

where \( \varepsilon \) is a white noise for the response. If the surface curvature exists, then the first-order polynomial model should be modified by adding the higher-order terms into this model. Therefore, at this time, the second-order polynomial model is employed for the surface approximation, i.e.

\[
y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i>j} \beta_{ij} x_i x_j + \varepsilon, \tag{1}
\]

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

The central composite design (CCD), initially proposed by Box and Wilson (1951), is the most popular design used for RSM. Basically a central composite design consists of a \( 2^k \) factorial (or a \( 2^{k-q} \) fractional factorial portion, of resolution \( V \) or higher), a set of \( 2k \) axial points at distances \( \alpha \) from the origin, and \( n_0 \) center points. The values of \( \alpha \) and \( n_0 \) need to be decided before the experiments. Usually \( \alpha \) can be chosen to be \( \sqrt{k} \). Then except the center points, all the other experimental points are on the surface of the \( k \)-ball with radius \( \sqrt{k} \), and this kind of CCD is called the spherical CCD. In CCD, the \( 2^k \) factorial (or a \( 2^{k-q} \) fractional factorial) design is used for fitting the first-order polynomial model, and then when the model changes to the second-order model, the axial points are added.
The weakness of the CCD’s is that the total number of the support points of CCD is extremely large, especially for large $k$. Hence when experimentations are time-consuming and very expensive, the small composite design should be a better choice. In previous works, to find small composite designs, they usually reduce the number of design points for fitting the first-order polynomial model and then add $2k$ axial points and one center point. Hence $2^k$ factorial (or $2^{k-q}$ fractional factorial) designs are replaced by the other small designs, for example: $2^k$ fractional factorial designs with resolution $III^*$ (Hartley, 1959), some irregular fractions of $2^k$ factorial designs (Westlake, 1965), and Plackett and Burman designs (Draper, 1985, and Draper and Lin, 1990). But these small composite designs still have more than $p$ experimental points. Thus in this thesis, we focus on the composite designs with minimal number of design points, and these designs are called the minimal-point designs.

Notz (1982) gave a definition of minimal-point design that a minimal-point design is one whose supports contain the minimal number of points such that the information matrix is nonsingular. Hence in this thesis, the minimal-point designs must satisfy the following two conditions:

**Condition (1)** the number of total design points is equal to $p$,

**Condition (2)** the corresponding information matrix is nonsingular.

To find the minimal-point designs, the two-stage procedure proposed by Chen, Lin and Tsai (2006) is used. Basically this procedure contains the two stages. The first stage is to find a proper first-order design and then remaining added points are selected in the second stage. Hence, these two stages are

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

**Stage 2** Add the remaining support points according to an optimal criterion over a design space.

In this thesis, the design, $\xi$, has $p$ trials at $p$ distinct points in design space $\mathcal{X}$, and
can be represented as

\[ \xi = \begin{pmatrix} x_1 & x_2 & \cdots & x_p \\ \frac{1}{p} & \frac{1}{p} & \cdots & \frac{1}{p} \end{pmatrix}, \]

where \( x_i \in \mathcal{X} \), \( i = 1, \ldots, p \), are the distinct supports of \( \xi \). Let \( X(\xi) \) be the \( p \times p \) model matrix of \( \xi \) and define \( \hat{\beta} \) to be the least-square estimator of the parameter vector \( \beta \) of the polynomial model. Then the covariance matrix of \( \hat{\beta} \) is equal to

\[ \text{Cov}(\hat{\beta}) = \sigma^2 (X(\xi)^\top X(\xi))^{-1} \propto (\frac{1}{p} X(\xi)^\top X(\xi))^{-1} = M^{-1}(\xi), \]

where \( M(\xi) = \frac{1}{p} X(\xi)^\top X(\xi) \) is the information matrix of \( \xi \). Generally we want to find a design \( \xi \) which minimize the covariance matrix in some senses, for instance, minimize the trace of the covariance matrix. Hence, in this thesis, the minimal-point designs would be constructed according to different optimal criteria. From two-stage method, our minimal-point designs are equal-weight designs and can be formulated as

\[ \xi = \frac{n_1 + 1}{p} \xi_1 + (1 - \frac{n_1 + 1}{p}) \xi_2 \] (2)

where \( \xi_1 \) is the design of the first-order portion and one center point; \( n_1 \) is the number of the support points of the first-order design, and \( \xi_2 \) is the equal-weight design with the \((p - n_1 - 1)\) distinct added support points. Due to the Condition (1), the support points of the first-order design, \( n_1 \), must be less than \( p - 1 \), because there is one center point.

This paper is organized as follows. In Section 2, the construction method for minimal-point designs is given, and a simulated annealing algorithm is introduced to find the remaining added points numerically. In Section 3, minimal-point designs based on different first-order designs are found. Then our minimal-point designs are compared with central composite designs and other small composite designs in Section 4. Finally a conclusion is given in Section 5.

## 2 Construction for Minimal-point Designs

This section is divided into two subsections according to the two-stage procedure. In Section 2.1, a restriction for the proper first-order designs is given, and then a numerical
method for selecting added support points is introduced in Section 2.2.

2.1 The restriction for first-order designs

In this subsection, we discuss what first-order designs should be in the two-stage procedure. Since the information matrix of the minimal-point design is nonsingular, we have the following theorem for choosing first-order designs. According to Equation (2), the second-order model matrix, \( X(\xi) \), is partitioned into two parts,

\[
X(\xi) = \begin{pmatrix}
X(\xi_1) \\
X(\xi_2)
\end{pmatrix},
\]

where \( X(\xi_1) \) is the \((n_1 + 1) \times p\) matrix with first-order design and one center point, and \( X(\xi_2) \) is the \((p - n_1 - 1) \times p\) matrix for added support points. Therefore we have the following theorem about the rank of \( X(\xi_1) \).

**Theorem 1.** Since the information matrix of minimal-point design is nonsingular, \( \xi_1 \) must satisfy that the rank of \( X(\xi_1) \) is equal to \( n_1 + 1 \).

**Proof:**

Due to the nonsingularity of the information matrix, we have

\[
\text{rank } X^\top(\xi) X(\xi) = \text{rank } X(\xi) = \text{rank } \begin{pmatrix} X(\xi_1) \\ X(\xi_2) \end{pmatrix} = p.
\]

Without loss of generality, we suppose the rows of \( X(\xi_1) \) and rows of \( X(\xi_2) \) are linearly independent. Thus, if \( \text{rank } X(\xi_1) < n_1 + 1 \), then it is clearly a contradiction. Because \( \text{rank } X(\xi) < p \), it induces that information matrix is singular. Hence we have the rank of \( X(\xi_1) \) must be equal to \( n_1 + 1 \). \( \square \)

In this thesis, the first-order designs are only focused on the 2-level designs. Therefore the first-order designs in Chen et al. (2006) are considered and are shown in Table 1. There are three types of 2-level designs, \( 2^k \) factorial designs (or \( 2^k \) fractional factorial designs with resolution V), \( 2^k \) fractional factorial designs with resolution III*, and Plackett and Burman designs.

Here, we need to check if the first-order designs in Table 1 are all satisfied the condition in Theorem 1. In fact, except the resolution V design with \( k = 3 \), all the other
<table>
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<tr>
<th>Factors, $k$</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
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<tr>
<td>Parameters</td>
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<td>10</td>
<td>15</td>
<td>21</td>
<td>28</td>
<td>36</td>
</tr>
<tr>
<td>Cube points $2^k(V)$</td>
<td>4</td>
<td>8</td>
<td>-</td>
<td>16</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Cube points $2^k(III^*)$</td>
<td>-</td>
<td>-</td>
<td>8</td>
<td>-</td>
<td>16</td>
<td>-</td>
</tr>
<tr>
<td>Cube points $2^k(PBD)$</td>
<td>-</td>
<td>4</td>
<td>8</td>
<td>11</td>
<td>16</td>
<td>22</td>
</tr>
</tbody>
</table>

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

cases are satisfied the condition in Theorem 1. For $k = 3$, when the first-order design is $2^3$ factorial design, we have

$$X(\xi_1) = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 & 1 \\
1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 & 1 \\
1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 \\
1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.
$$

Because there are three identical columns in $X(\xi_1)$, the rank of $X(\xi_1)$ must be less than 9. Hence it is a contradict with the condition in Theorem 1, and this design can not be the first-order design under our construction method. Thus in this thesis, we consider designs in Table 1 except $2^3$ factorial design to be our first-order designs.

### 2.2 The numerical method for finding added support points

Given a proper first-order design, we need to find the added points to form the minimal-point second-order response surface design. In Chen et al. (2006), these added points are chosen from the design space according to an optimal criterion. The design space for the case of $k$ factors is the sphere with radius $\sqrt{k}$, i.e. $\mathcal{X} = \{(x_1, \ldots, x_k) | x_1^2 +
\[\cdots + x_k^2 \leq k\},\] because we follow the same structure of spherical CCD’s. In Chen et al. (2006), only \(D\)-optimal criterion is used for selecting points. In this thesis, we consider three criteria: \(A\) - and \(A_s\)-optimal criteria and slope-rotatable criterion. Here, \(A\) - and \(A_s\)-optimal criteria are useful to measure the performance of estimation of the parameters, and slope-rotatable criterion is related to the information of predictions throughout the region of interest. The details about these criteria are described in next section.

Due to spherical design space, it is a good idea to represent these added support points by polar coordinate or spherical coordinate. For example, when \(k = 2\), our minimal-point design contains \(2^2\) factorial points, one center point, and one added point. Thus this added support point is represented by

\[(x_{11}, x_{12}) = (r_1 \cos \theta_{11}, r_1 \sin \theta_{11}),\]

where \(0 < r_1 \leq \sqrt{2},\) \(0 \leq \theta_{11} < 2\pi\). Hence \(X(\xi)\) is

\[
X(\xi) = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & -1 & -1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 & 1 & 1 \\
1 & -1 & -1 & 1 & 1 & 1 & 1 \\
1 & r_1 \cos \theta_{11} & r_1 \sin \theta_{11} & r_1^2 \sin \theta_{11} \cos \theta_{11} & r_1^2 \cos \theta_{11}^2 & r_1^2 \sin \theta_{11}^2 \\
1 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.
\]

This representation can be easy extended to the general cases. As a first-order design and one center point are given, there are still \(p - n_1 - 1\) remaining support points. Applying the spherical coordinate, the coordinates of these remaining points are represented as

\[x_i = (x_{i1}, x_{i2}, x_{i3}, \ldots, x_{ik}) \quad , i = 1, \ldots, (p - n_1 - 1),\]

where

\[x_{i1} = r_i \sin \theta_{i(k-1)} \cdots \sin \theta_{i2} \cos \theta_{i1};\]
\[x_{i2} = r_i \sin \theta_{i(k-1)} \cdots \sin \theta_{i2} \sin \theta_{i1};\]
\[x_{i3} = r_i \sin \theta_{i(k-1)} \cdots \sin \theta_{i3} \cos \theta_{i2};\]
\[ x_{ik} = r_i \cos \theta_{i(k-1)}, \]

and \( 0 < r_i \leq \sqrt{k}; \ 0 \leq \theta_{ij} < 2\pi. \) Hence the information matrix of \( \xi \) now is a function of \( r_i \) and \( \theta_{ij} \). For simplicity, we use \( \theta_1, \ldots, \theta_q \) to index all the angles. Let \( r = (r_1, \ldots, r_{p-n_1-1}) \) and \( \theta = (\theta_1, \ldots, \theta_q) \). Define \( d(r, \theta) \) to be the objective function of \( X^\top(\xi)X(\xi) \). For example, when A-optimal criterion is used, the objective function is

\[ Tr(X^\top(\xi)X(\xi))^{-1}. \]

Hence, to find our minimal-point design is to minimize the objective function directly with respect to \( r \) and \( \theta \). However \( d(r, \theta) \) may be too complicated to write down its close form, especially when \( k \) is large. Thus the Best Angle and Radius (BAR) algorithm, proposed by Chen et al. (2006), is used to find the minimum of \( d(r, \theta) \) numerically.

Basically the BAR algorithm is a simulated annealing (SA) type algorithm (Metropolis et al., 1953, and Kirkpatrick et al., 1983) to optimize \( d(r, \theta) \) with respect to \( r \) and \( \theta \). Since the objective function is \( d(r, \theta) \) that we want to minimize, we denote a density \( \pi_{T(t)}(r, \theta) \) in our BAR sampler to be

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

where \( T(t) \) is the “temperature” at time \( t \) and is a decreasing function from initial temperature, \( T(0) > 0, \) to 0+. Then BAR sampler is in the following:

**Step 1.** Select the initial angles, \( \theta_j^{(0)}, \ j = 1, \ldots, q, \) and initial radiuses, \( r_i^{(0)}, \ i = 1, \ldots, p-n_1-1, 0 < r_i^{(0)} \leq \sqrt{k}; \ 0 \leq \theta_j^{(0)} < 2\pi. \)

**Step 2.** Run \( N_t \) iterations of the Gibbs sampler to sample \( r \) and \( \theta \) from \( \pi_{T(t)}(r, \theta) \), and at each iteration of the Gibbs sampler,

1. Sampler \( r_i, \ i = 1, \ldots, p-n_1-1, \) from \( \pi_{T(t)}(r_i \mid r_{-i}, \theta) \)
2. Draw \( \theta_j, \ j = 1, \ldots, q, \) from \( \pi_{T(t)}(\theta_j \mid r, \theta_{-j}) \)

by the inversion method.
Step 3. Set \( t \) to \( t + 1 \), go to step 2 until \( t \) is large enough.

In Gibbs sampler, \( r_{-i} \) is a set of all radiuses \( r_m \) except the \( i^{th} \) radius and \( \theta_{-j} \) is a set of all angles \( \theta_m \) except the \( j^{th} \) angle, i.e. \( r_{-i} = (r_1, \ldots, r_{i-1}, r_{i+1}, \ldots, r_{p-n_1-1}) \) and \( \theta_{-j} = (\theta_1, \ldots, \theta_{j-1}, \theta_{j+1}, \ldots, \theta_q) \). Since the SA algorithm can only find the local extreme values and may be affected by the initial states, we would choose the initial angles and radiuses randomly. We also check the tendency of objective function \( d(r, \theta) \) of BAR sampler to make sure that \( d(r, \theta) \) is close to an extreme value.

3 Minimal-point Designs

Applying our construction method, the minimal-point designs are found according to different criteria. As mentioned before, two types of criteria are chosen here, one is about the parameter estimates, and another one is about prediction. Thus this section is divided into two parts according to these two types of criteria. \( A \)- and \( A_s \)-optimal minimal-point designs are shown in Section 3.1 and in Section 3.2, the slope-rotatable criterion is considered.

3.1 \( A \)- and \( A_s \)-optimal minimal-point composite designs

In \( A \)-optimality, \( Tr\{M^{-1}(\xi)\} \), the average variance of the parameter estimates, is minimized. Hence when \( A \)-optimal criterion is considered, the objective function is defined as

\[
d_{A,k}(r, \theta) = Tr(X^\top(\xi)X(\xi))^{-1}.
\]

In \( A \)-optimal criterion, the performance of all parameters in the model are considered. However, we may not be interested in whole parameters. Following Section 2.10 in Fedorov (1972), we consider the \( A_s \)-optimal criterion. In \( A_s \)-optimality, the parameters of the second-order terms and interaction terms are treated as the parameters of interest, and the parameters in the first-order model are the nuisance parameters. Therefore, the
model is divided into two groups:

\[ E(y) = f_1^\top(x) \beta_1 + f_2^\top(x) \beta_2, \]

where \( f_1(x) = (1, x_1, \ldots, x_k)^\top; \) \( \beta_1 = (\beta_0, \beta_1, \ldots, \beta_k)^\top; \) \( f_2(x) \) contains all second-order terms and interaction terms, \( x_i^2 \) and \( x_ix_j, \) and \( \beta_2 \) is the parameter vector of the corresponding parameters of interest, \( \beta_{ij}, 1 \leq i \leq j \leq k. \) According to Equation (2), we can divide the information matrix into four parts

\[ M(\xi) = \begin{pmatrix} M_{11}(\xi) & M_{12}(\xi) \\ M_{12}^\top(\xi) & M_{22}(\xi) \end{pmatrix}, \]

where \( M_{11}(\xi) \) is the information matrix for \( \beta_1 \) and \( M_{22}(\xi) \) is the information matrix for \( \beta_2. \) Define

\[
\bar{X}_{22}(\xi) = \begin{pmatrix} 0 & \cdots & 0 & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & 1 \end{pmatrix} \begin{pmatrix} M_{11}(\xi) & M_{12}(\xi) \\ M_{12}^\top(\xi) & M_{22}(\xi) \end{pmatrix}^{-1} \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \\ 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{pmatrix} = (0 \ I) M^{-1}(\xi) \begin{pmatrix} 0 \\ I \end{pmatrix}.
\]

Thus a design \( \xi^* \) is \( A_s \)-optimality if

\[ \xi^* = \arg\min_{\xi} Tr(\bar{X}_{22}(\xi)) \]

Hence the objective function for \( A_s \)-optimality is

\[ d_{A_s,k}(r, \theta) = Tr(0 \ I)(X^\top(\xi)X(\xi))^{-1} \begin{pmatrix} 0 \\ I \end{pmatrix} = Tr(\bar{M}_{22}(\xi)). \]

For the cases of \( k = 2, \ldots, 7, \) the minimal-point composite designs for \( A \)- and \( A_s \)-optimal criteria are shown, and we denote \( \xi_{A,k} \) and \( \xi_{A_s,k} \) to be the minimal-point designs for \( k \) factors found by \( A \)- and \( A_s \)-optimal criteria.
3.1.1 $A$- and $A_s$-optimal minimal-point composite designs for $k = 2$

For the case of $k = 2$, the first-order design is the $2^2$ factorial design. Since there are 6 parameters in the second-order polynomial model, we need to add one more support point to form a minimal-point design. This added support point is represented by polar coordinate, i.e.

$$(x_{11}, x_{12}) = (r_1 \cos \theta_{11}, r_1 \sin \theta_{11}),$$  \hspace{1cm} \text{(3)}$$

where $0 < r_1 \leq \sqrt{2}, \ 0 \leq \theta_{11} < 2\pi$.

- $A$-optimal criterion

Since there is only one added point, we have the following lemma to show the trace of $(X^\top(\xi)X(\xi))^{-1}$.

**Lemma 1.** When $k = 2$, based on the $2^2$ factorial design, the trace of inverse of the information matrix is proportional to

$$Tr(X^\top(\xi)X(\xi))^{-1} = \frac{9}{4} + \frac{1}{4} \left(3 + \frac{16}{r_1^2} - \frac{6}{r_1^2} \sec[2\theta_{11}]^2 \right).$$

When $\theta_{11} = 0$, the minimum value of $\sec[2\theta_{11}]^2$ is 1, and then $Tr(X^\top(\xi)X(\xi))^{-1}$ is a decreasing function with respected to $r_1$. Thus, the minimum value is attended at $\theta_{11} = 0$ and $r_1 = \sqrt{2}$. Hence the added support point is $(\sqrt{2}, 0)$, and the corresponding trace is 3.2500.

Now we would apply the BAR sampler to find the result numerically. With a random initial state, we set $T(t) = (5t)^{-2/3}$ and the iteration number of Gibbs sampling, $N_t$, is set to be 10. Totally our algorithm is iterated 2500 times. The optimal added support point found by BAR sampler is

$$\begin{pmatrix} 1.4142 & 0.0001 \end{pmatrix}.$$

This point is very close to the axial point of the spherical CCD of two factors and the value of the trace of $(X^\top(\xi_{A,2})X(\xi_{A,2}))^{-1}$ is 3.2500. In fact, we can show that the added support point can be any one of four axial points. Figure 1 displays the tendency of the trace of $(X^\top(\xi)X(\xi))^{-1}$ in BAR sampler.
• \( A_s \)-optimal criterion

Under our design structure, we have the following lemma for \( Tr(\bar{M}_{22}(\xi)) \).

**Lemma 2.** When \( k = 2 \), based on the \( 2^2 \) factorial design, the trace of \( \bar{M}_{22}(\xi) \) is proportional to

\[
Tr(\bar{M}_{22}(\xi)) \propto \frac{3}{4} + \frac{1}{4} (3 + \frac{16}{r_1^4} - \frac{6}{r_1^2}) \sec[2\theta_{11}]^2.
\]

It is easy to show that the minimum value of \( Tr(\bar{M}_{22}(\xi)) \) is attended when \( \theta_{11} = 0 \) and \( r_1 = \sqrt{2} \). Hence the corresponding support point is \((\sqrt{2}, 0)\). At this time, the value of \( Tr(\bar{M}_{22}(\xi)) \) is 1.7500.

We also use the BAR sampler to find this added point. We suppose \( T(t) = (5t)^{-2/3} \) and \( N_t = 10 \). After 2500 iterations of BAR sampler, the optimal added support point is

\[
\begin{pmatrix}
0.0001 \\
1.4142
\end{pmatrix}
\]

and the optimal value is 1.7500. The numerical result shows that the added support point is close to axial point. In fact, the added support point for \( A_s \)-optimal minimal-point design is any one of four axial points. Figure 2 displays the tendency of the trace of \( \bar{M}_{22}(\xi) \).
Figure 2: For $k=2$, the trace of $A_s$-optimal criterion for $2500 \times 10 = 25000$ steps.

From above results, we get the same added support point for $A$- and $A_s$-optimal criteria. Hence for $k = 2$, $A$- and $A_s$-optimal minimal-point designs are equal to each other.

3.1.2 $A$- and $A_s$-optimal minimal-point composite designs for $k = 3$

For $k = 3$, the first-order design is chosen from the column $(1, 2, 3)$ of 4-runs $P-B$ design, and the design space is the 3-ball with radius $\sqrt{3}$. Since there are 10 parameters in the second-order polynomial model, five added support points are required for a minimal-point second-order design. The coordinates of these added points are written as

$$x_i = (x_{i1}, x_{i2}, x_{i3}),$$

where $x_{i1} = r_i \sin \theta_{i2} \cos \theta_{i1}$, $x_{i2} = r_i \sin \theta_{i2} \sin \theta_{i1}$ and $x_{i3} = r_i \cos \theta_{i2}$, $i = 1, \ldots, 5$.

- $A$-optimal criterion

We find the $A$-optimal added points by the BAR sampler with $T(t) = (3t)^{-2/3}$ and $N_t = 10$. After 2500 iterations, the minimum value of $Tr(X^T(\xi_{A,3})X(\xi_{A,3}))^{-1}$ is
2.8788 and $A$-optimal added support points are

$$
\begin{bmatrix}
0.1497 & 1.5137 & 0.8285 \\
-1.5232 & -0.1838 & 0.8039 \\
1.4401 & 0.6298 & 0.7276 \\
-0.0586 & 0.0701 & 1.7296 \\
-0.6295 & -1.4524 & 0.7031
\end{bmatrix}
$$

In fact, the radiuses of the five added points are all close to $\sqrt{3}$.

- $A_s$-optimal criterion

The BAR sampler is also used to find the $A_s$-optimal support points. Here we assume $T(t) = (5t)^{-2/3}$ and $N_t$ is set to be 10. Totally our algorithm is iterated 2500 times, and the $A_s$-optimal added support points are

$$
\begin{bmatrix}
-0.6990 & -1.4367 & 0.6689 \\
-1.5363 & -0.1270 & 0.7897 \\
-0.0892 & 0.0877 & 1.7275 \\
1.4386 & 0.6649 & 0.6988 \\
0.1330 & 1.5292 & 0.8025
\end{bmatrix}
$$

The corresponding optimal value is 1.3545 and those five radiuses are also close to $\sqrt{3}$.

Here we find that $A$- and $A_s$-optimal minimal-point designs for $k = 3$ are similar to each other from the following table.

<table>
<thead>
<tr>
<th>$\xi_{A,3}$</th>
<th>$Tr(X^\top(\xi)X(\xi))^{-1}$</th>
<th>$Tr(\tilde{M}_{22}(\xi))$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.8788</td>
<td>2.8800</td>
<td>1.3545</td>
</tr>
</tbody>
</table>

### 3.1.3 $A$- and $A_s$-optimal minimal-point composite designs for $k = 4$

For $k = 4$, the design space is the 4-ball with radius 2, and there are 15 parameters in the second-order polynomial model. The first-order design is the $2^{4-1}$ fractional factorial
design with resolution $III^*$ proposed by Hartley (1959). Hence six added support points are required for a minimal-point design, and coordinates of these added points are

$$x_i = (x_{i1}, x_{i2}, x_{i3}, x_{i4}),$$

where $x_{i1} = r_i \sin \theta_{i3} \sin \theta_{i2} \cos \theta_{i1}$, $x_{i2} = r_i \sin \theta_{i3} \sin \theta_{i2} \sin \theta_{i1}$, $x_{i3} = r_i \sin \theta_{i3} \cos \theta_{i2}$ and $x_{i4} = r_i \cos \theta_{i3}$, $i = 1, \ldots, 6$.

- **A-optimal criterion**

Here we use the BAR sampler to find the $A$-optimal added points with $T(t) = (20t)^{-2/3}$ and $N_t = 10$. After 2500 iterations, the $A$-optimal added supports we get are

$$
\begin{bmatrix}
0.4429 & -1.3189 & 1.4327 & -0.1080 \\
-0.4592 & -1.3016 & -1.4431 & -0.1109 \\
0.0000 & 1.9978 & 0.0198 & -0.0923 \\
0.5110 & 0.8565 & -1.7305 & -0.1037 \\
-0.0001 & -0.0003 & -0.0078 & 2.0000 \\
-0.5261 & 0.8316 & 1.7375 & -0.1119
\end{bmatrix}.
$$

The trace of $(X^\top (\xi_{A,4}) X(\xi_{A,4}))^{-1}$ is 2.8612 and those six radiuses, $r_1, \ldots, r_6$, are close to the boundary 2.

- **$A_s$-optimal criterion**

Applying our BAR sampler searches out the $A_s$-optimal added supports with the assumptions, $T(t) = (5t)^{-2/3}$ and $N_t = 10$. After 2500 iterations, the minimum trace of $\bar{M}_{22}(\xi_{A_s,4})$ is 1.4631, and the $A_s$-optimal added support points found by BAR sampler are

$$
\begin{bmatrix}
1.7734 & 0.4462 & -0.8040 & -0.0981 \\
0.0023 & 0.0007 & 0.0025 & 2.0000 \\
-1.7853 & -0.4336 & -0.7816 & -0.1175 \\
-0.0556 & 0.0010 & -1.9917 & -0.1737 \\
-1.4326 & 0.3875 & 1.3248 & -0.2058 \\
1.4235 & -0.4124 & 1.3321 & -0.1703
\end{bmatrix}.
$$
The numerically result is that the six radiuses, \( r_i, \ i = 1, \ldots, 6 \), are close to 2.

We can follow the same process of case \( k = 3 \), then a table is given below

<table>
<thead>
<tr>
<th>( \xi_{A,4} )</th>
<th>( Tr(X^\top(\xi)X(\xi))^{-1} )</th>
<th>( Tr(\bar{M}_{22}(\xi)) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.8612</td>
<td>1.4688</td>
<td></td>
</tr>
<tr>
<td>2.8702</td>
<td>1.4631</td>
<td></td>
</tr>
</tbody>
</table>

Hence we regard that \( A \)- and \( A_s \)-optimal minimal-point designs are similar to each other for \( k = 4 \).

### 3.1.4 \( A \)- and \( A_s \)-optimal minimal-point composite designs for \( k = 5 \)

There are two first-order designs for \( k = 5 \), one is the \( 2^5-1 \) fractional factorial design with resolution \( V \) and the other one is Plackett and Burman design with \( k = 5 \). There are 21 unknown parameters in the second-order polynomial model and the design space is the 5-ball with radius \( \sqrt{5} \).

#### \( 2^5-1 \) fractional factorial design with resolution \( V \)

Since the first-order design is the \( 2^5-1 \) fractional factorial design with resolution \( V \), four added support points are required for a minimal-point second-order design, and the coordinates of these four added points are

\[
x_i = (x_{i1}, x_{i2}, x_{i3}, x_{i4}, x_{i5}),
\]

where

\[
x_{i1} = r_i \sin \theta_{i4} \sin \theta_{i3} \sin \theta_{i2} \cos \theta_{i1}, \quad x_{i2} = r_i \sin \theta_{i4} \sin \theta_{i3} \sin \theta_{i2} \sin \theta_{i1},
\]

\[
x_{i3} = r_i \sin \theta_{i4} \sin \theta_{i3} \cos \theta_{i2}, \quad x_{i4} = r_i \sin \theta_{i4} \cos \theta_{i3} \quad \text{and} \quad x_{i5} = r_i \cos \theta_{i4}, \ i = 1, \ldots, 4.
\]

#### \( A \)-optimal criterion

We use the BAR sampler to find \( A \)-optimal radiuses, \( r_1, \ldots, r_4 \), and angles, \( \theta_{ij} \).

Here we assume \( T(t) = (20t)^{-2/3} \) and \( N_t = 10 \). Totally our algorithm is iterated 2500 times. The \( A \)-optimal added support points that we get are

\[
\begin{bmatrix}
0.0058 & -0.1050 & -0.0571 & \mathbf{2.2305} & -0.1018 \\
-0.0084 & -0.0886 & -0.0734 & -0.0717 & \mathbf{2.2319} \\
0.0092 & \mathbf{2.2287} & -0.1095 & -0.1052 & -0.0993 \\
-0.0110 & -0.0526 & \mathbf{2.2307} & -0.1082 & -0.0958
\end{bmatrix}
\]
and the trace of $\left(X^\top(\xi_{A,5})X(\xi_{A,5})\right)^{-1}$ is 2.6142. Those radiuses of the four added support points are all close to $\sqrt{5}$. Because these added supports are close to axial points, $(0, 0, 0, \sqrt{5}, 0), (0, 0, 0, 0, \sqrt{5}), (0, \sqrt{5}, 0, 0, 0)$ and $(0, 0, \sqrt{5}, 0, 0)$, we replace the $A$-optimal added points with these four axial points. However, the trace of this new design is 2.6200. Thus, these axial points can not be our $A$-optimal added points.

- $A_s$-optimal criterion

Here we still use BAR sampler to find the $A_s$-optimal added points with $T(t) = (20t)^{-2/3}$ and $N_t = 10$. After 2500 iterations, those four radiuses are also close to $\sqrt{5}$, and the added support points are

$$\begin{bmatrix}
-0.0037 & -0.0521 & -0.0853 & 2.2318 & -0.0956 \\
-0.0074 & -0.0657 & -0.0908 & -0.0953 & 2.2312 \\
-0.0119 & 2.2281 & -0.0814 & -0.1209 & -0.1195 \\
-0.0031 & -0.0998 & 2.2290 & -0.1063 & -0.1021
\end{bmatrix}.$$  

The trace of $\bar{M}_{22}(\xi_{A,s})$ is 1.3017. We obtain that those added support points are also close to the axial points, $(0, 0, \sqrt{5}, 0, 0), (0, 0, 0, \sqrt{5}, 0), (0, 0, 0, 0, \sqrt{5})$ and $(\sqrt{5}, 0, 0, 0, 0)$. Hence we replace the $A_s$-optimal added points with these four axial points. However the trace of this new design is 1.3075. It indicates that these axial points can not be our $A_s$-optimal added support points.

The table given below is to compare $A$- and $A_s$-optimal minimal-point designs.

<table>
<thead>
<tr>
<th></th>
<th>$Tr(X^\top(\xi)X(\xi))^{-1}$</th>
<th>$Tr(\bar{M}_{22}(\xi))$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\xi_{A,5}$</td>
<td>2.6142</td>
<td>1.3017</td>
</tr>
<tr>
<td>$\xi_{A,s,5}$</td>
<td>2.6142</td>
<td>1.3017</td>
</tr>
</tbody>
</table>

We can obtain that $A$- and $A_s$-optimal minimal-point designs are equal to each other when the first-order design is $2^{5-1}$ factional factorial design with resolution $V$.

**Plackett and Burman design for $k = 5$**

In this part, the first-order design is the columns $(1, 2, 3, 5, 8)$ from 12-runs $P-B$ design without run 11. Since there are 21 parameters in the model, we have 11 support
points in the first-order design and 9 added support points are required for a minimal-point second-order design. The coordinates of these added points are

\[ x_i = (x_{i1}, x_{i2}, x_{i3}, x_{i4}, x_{i5}), \]

where \( x_{i1} = r_i \sin \theta_{i1} \sin \theta_{i2} \cos \theta_{i1}, \) \( x_{i2} = r_i \sin \theta_{i1} \sin \theta_{i2} \sin \theta_{i1}, \)
\( x_{i3} = r_i \sin \theta_{i1} \sin \theta_{i3} \cos \theta_{i2}, \) \( x_{i4} = r_i \sin \theta_{i4} \sin \theta_{i3} \sin \theta_{i1}, \) and \( x_{i5} = r_i \cos \theta_{i4}, \) \( i = 1, \ldots, 9. \)

**A-optimal criterion**

Our BAR sampler are applied to find the added points of A-optimal criterion with the assumptions, \( T(t) = (20t)^{-2/3} \) and \( N_t = 10. \) Totally our algorithm is iterated 2500 times, and the A-optimal added support points found by BAR sampler are

\[
\begin{bmatrix}
-0.7848 & -0.6930 & -1.4810 & -0.7144 & 1.0956 \\
0.2946 & 1.9709 & 0.8986 & 0.3567 & 0.3070 \\
-0.4273 & -0.3990 & 2.0797 & -0.4110 & -0.4052 \\
2.0008 & 0.3002 & 0.8657 & 0.2726 & 0.2878 \\
-0.7139 & 1.0786 & -1.4862 & -0.7466 & -0.7488 \\
0.3239 & 0.2724 & 0.8439 & 2.0041 & 0.3041 \\
1.0031 & -0.6832 & -1.5584 & -0.7594 & -0.7223 \\
0.2701 & 0.2641 & 0.7774 & 0.3041 & 2.0397 \\
-0.6906 & -0.7125 & -1.5522 & 1.0299 & -0.7385
\end{bmatrix}
\]

The trace of \( (X^\top(\xi_{A,5})X(\xi_{A,5}))^{-1} \) is 2.6461 and those radiuses, \( r_1, \ldots, r_9, \) are all close to the boundary \( \sqrt{5}. \)

**A_s-optimal criterion**

Our BAR sampler is reapplied, we can find the \( A_s \)-optimal radiuses, \( r_1, \ldots, r_9, \) and angles, \( \theta_{ij}. \) Here we assume \( T(t) = (20t)^{-2/3} \) and \( N_t = 10. \) After 2500 iterations, the minimum value of \( Tr(\bar{M}_{22}(\xi_{A_s,5})) \) is 1.2797 and the \( A_s \)-optimal added support
The radiuses of those nine added support points are also close to $\sqrt{5}$.

From the following table, when the first-order design is $P$-$B$ design for $k = 5$, it seems that $A$- and $A_s$-optimal minimal-point designs are similar to each other.

<table>
<thead>
<tr>
<th></th>
<th>$Tr(X\top(\xi)X(\xi))^{-1}$</th>
<th>$Tr(\bar{M}_{22}(\xi))$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\xi_{A,5}$</td>
<td>2.6461</td>
<td>1.2870</td>
</tr>
<tr>
<td>$\xi_{A_s,5}$</td>
<td>2.6574</td>
<td>1.2797</td>
</tr>
</tbody>
</table>

### 3.1.5 $A$- and $A_s$-optimal minimal-point composite designs for $k = 6$

For $k = 6$, the design space is the 6-ball with radius $\sqrt{6}$. The first-order design is the $2^{6-2}$ fractional factorial design with resolution $III^*$, and there are 28 unknown parameters in the second-order polynomial model. Therefore, 11 added supports are required to form our minimal-point design. However from the above numerical results, the radiuses of those added support points are all close to the boundary $\sqrt{k}$. In order to simplify our algorithm, we assume one radius for all those added points to find the optimal added support points, i.e. all added points have the same radius, $r$. Hence the coordinates of these points are represented as

$$x_i = (x_{i1}, x_{i2}, x_{i3}, x_{i4}, x_{i5}, x_{i6})$$
where \( x_{i1} = r \sin \theta_{i5} \sin \theta_{i4} \sin \theta_{i3} \sin \theta_{i2} \cos \theta_{i1} \), \( x_{i2} = r \sin \theta_{i5} \sin \theta_{i4} \sin \theta_{i3} \sin \theta_{i2} \cos \theta_{i1} \), \( x_{i3} = r \sin \theta_{i5} \sin \theta_{i4} \sin \theta_{i3} \cos \theta_{i2} \), \( x_{i4} = r \sin \theta_{i5} \sin \theta_{i4} \cos \theta_{i3} \), \( x_{i5} = r \sin \theta_{i5} \cos \theta_{i4} \) and \( x_{i6} = r \cos \theta_{i5} \), \( i = 1, \ldots, 11 \).

- **A-optimal criterion**

Our BAR sampler is applied for finding the added support points of A-optimal criterion. Here we assume \( T(t) = (5t)^{-2/3} \) and \( N_t = 10 \). After 1500 iterations, the minimum trace of \( (X^T(\xi_{A,6})X(\xi_{A,6}))^{-1} \) is 2.5721, and the A-optimal added supports points we get are

\[
\begin{bmatrix}
1.3514 & 1.4196 & -1.4670 & 0.0194 & -0.0185 & 0.0750 \\
0.4245 & -0.4508 & 2.3680 & -0.0495 & 0.0473 & -0.0659 \\
0.3837 & -2.3764 & 0.4139 & 0.1060 & 0.1338 & 0.0718 \\
2.3632 & -0.5096 & 0.3716 & -0.0190 & -0.0993 & -0.0858 \\
0.0330 & -0.0401 & 0.0231 & -0.7718 & -1.0709 & -2.0626 \\
0.0229 & 0.0208 & -0.0970 & -0.0520 & -2.4437 & -0.1228 \\
0.0008 & -0.0002 & -0.0219 & 0.6599 & -1.1580 & 2.0550 \\
-1.4002 & 1.5580 & 1.2664 & 0.0096 & 0.0553 & -0.0710 \\
-0.0089 & 0.0129 & -0.0551 & 0.5769 & 1.5346 & -1.8190 \\
-1.4534 & -1.2937 & -1.4688 & -0.0387 & 0.1216 & 0.2005 \\
-0.0012 & 0.0018 & 0.0035 & -0.5573 & 1.6149 & 1.7554
\end{bmatrix}
\]

Here the radius, \( r \), is close to \( \sqrt{6} \).

- **\( A_s \)-optimal criterion**

Here we reapply the BAR sampler to find the \( A_s \)-optimal added points with \( T(t) = (5t)^{-2/3} \) and \( N_t = 10 \). Totally our algorithm is iterated 1500 times. The minimum value of \( Tr(\hat{M}_{22}(\xi_{A,s})) \) is 1.3000, and the \( A_s \)-optimal added support points found
by BAR sampler are
\[
\begin{pmatrix}
-0.6964 & 0.7162 & 2.2362 & 0.0280 & 0.0061 & -0.0260 \\
1.4077 & 0.4679 & -1.9435 & 0.0384 & 0.0487 & 0.1358 \\
0.0129 & 0.0144 & 0.0873 & -1.4733 & 1.3537 & 1.4103 \\
0.0007 & -0.0002 & -0.0728 & 2.4362 & -0.1701 & 0.1747 \\
0.0029 & 0.0020 & 0.0046 & 1.2338 & 1.5556 & -1.4345 \\
1.4984 & -0.4228 & 1.8890 & -0.0697 & 0.0515 & 0.0150 \\
-1.2627 & -0.6532 & -1.9868 & 0.1765 & -0.0167 & 0.0118 \\
-2.4431 & 0.0965 & 0.1188 & 0.0772 & 0.0045 & 0.0454 \\
0.0135 & 0.0611 & 0.0287 & 0.4981 & -0.2082 & 2.3883 \\
0.0083 & -0.0057 & -0.0113 & -1.3089 & -1.4651 & -1.4628 \\
-0.0001 & -0.0008 & 0.0053 & 0.4876 & -2.3823 & 0.2951 \\
\end{pmatrix}
\]

The only one radius is also close to $\sqrt{6}$.

From the following table, we conclude that $A$- and $A_s$-optimal minimal-point designs are similar to each other for $k = 6$.

<table>
<thead>
<tr>
<th>$\xi_{A,6}$</th>
<th>$Tr(X^\top(\xi)X(\xi))^{-1}$</th>
<th>$Tr(\tilde{M}_{22}(\xi))$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\xi_{A,6}$</td>
<td>2.5721</td>
<td>1.3033</td>
</tr>
<tr>
<td>$\xi_{A_s,6}$</td>
<td>2.5867</td>
<td>1.3000</td>
</tr>
</tbody>
</table>

3.1.6 $A$- and $A_s$-optimal minimal-point composite designs for $k = 7$

For $k = 7$, there are 36 parameters in the second-order polynomial model. The first-order design is to choose the columns (1, 2, 5, 6, 7, 9, 10) from 24-runs $P$-$B$ design without run 3 and run 20. Hence the first-order design has 22 supports, and we need to add 13 support points to form the minimal-point design. We also follow the same structure of case for $k = 6$, only one radius is used for these added support points. Hence the 13 added points are represented by the coordinates as

$$x_i = (x_{i1}, x_{i2}, x_{i3}, x_{i4}, x_{i5}, x_{i6}, x_{i7}),$$
where $x_{i1} = r \sin \theta_{i6} \sin \theta_{i5} \sin \theta_{i4} \sin \theta_{i3} \cos \theta_{i1}$, $x_{i2} = r \sin \theta_{i6} \sin \theta_{i5} \sin \theta_{i4} \sin \theta_{i2} \sin \theta_{i1}$, $x_{i3} = r \sin \theta_{i6} \sin \theta_{i5} \sin \theta_{i4} \cos \theta_{i2}$, $x_{i4} = r \sin \theta_{i6} \sin \theta_{i5} \sin \theta_{i4} \cos \theta_{i3}$, $x_{i5} = r \sin \theta_{i6} \sin \theta_{i5} \cos \theta_{i4}$, $x_{i6} = r \sin \theta_{i6} \cos \theta_{i5}$ and $x_{i7} = r \cos \theta_{i6}$, $i = 1, \ldots, 13$.

- **$A$-optimal criterion**

  we employ the BAR sampler to find the $A$-optimal radius and angles. We suppose $T(t) = (20t)^{-2/3}$ and set $N_t = 10$. After 1500 iterations, the $A$-optimal added support points are

  $\begin{bmatrix}
  -0.0163 & -0.2887 & 0.8332 & -0.4317 & 2.4125 & 0.4370 & 0.1570 \\
  -0.9724 & -0.7355 & 0.6709 & -0.1525 & 0.9745 & -1.6263 & -1.2023 \\
  0.3682 & 0.0294 & 2.4752 & 0.1401 & 0.8055 & -0.2575 & -0.0445 \\
  0.4890 & -0.3300 & -1.4823 & 0.8098 & -0.8381 & -0.7552 & 1.5894 \\
  -1.4529 & -0.4572 & -0.6276 & 1.0570 & -1.4953 & 0.8141 & -0.5199 \\
  0.4961 & -2.4764 & 0.1771 & -0.6620 & -0.0080 & -0.3893 & 0.0092 \\
  0.2571 & 0.1597 & 0.0080 & -0.5262 & 0.4961 & 2.4699 & -0.5337 \\
  -0.3906 & 0.2477 & 0.4033 & -1.0184 & 0.8664 & -1.4955 & 1.6122 \\
  0.2087 & 0.5828 & -0.1490 & 2.5386 & -0.3093 & -0.0459 & 0.2282 \\
  -1.3389 & 0.2484 & 0.4451 & 0.2020 & 0.3127 & 1.5671 & 1.5339 \\
  -0.2736 & 1.1669 & -0.0177 & 0.9018 & 1.1695 & 0.5645 & -1.7503 \\
  0.4387 & -0.6091 & 0.9076 & -0.2231 & -0.4885 & 0.2010 & -2.2987 \\
  2.4880 & -0.7155 & 0.0927 & 0.3967 & 0.2839 & 0.1701 & 0.1504 
  \end{bmatrix}$

  The minimum trace of $(X^\top (\xi_{A7}) X (\xi_{A7}))^{-1}$ is 3.3109 and the radius is close to $\sqrt{7}$.

- **$A_s$-optimal criterion**

  Our BAR sampler is used to find the $A_s$-optimal added supports points with supposition $T(t) = (20t)^{-2/3}$ and $N_t = 10$. Totally our algorithm is iterated 1500 times,
and the $A$-optimal added support points are

$$
\begin{bmatrix}
-0.2079 & -1.4002 & 1.1925 & -0.8416 & 0.6387 & -0.7760 & -1.3623 \\
-0.1122 & 2.4421 & 0.4831 & 0.7393 & 0.3286 & 0.1466 & -0.3373 \\
-0.2521 & 0.3870 & 0.6533 & -1.0715 & 0.9376 & -1.4236 & 1.5185 \\
-1.3979 & -0.5945 & -0.1835 & 1.0828 & -1.4156 & 0.6702 & -1.0164 \\
-0.3314 & 0.4069 & -0.1266 & 0.0437 & -0.1336 & 2.5835 & -0.1192 \\
-0.0571 & 0.6237 & 0.1875 & 2.5580 & 0.0496 & 0.1199 & -0.1108 \\
0.4549 & -0.6451 & -1.4058 & 0.6785 & -0.9587 & -0.7857 & 1.5504 \\
-1.1943 & -0.3851 & -0.3696 & 0.4819 & 1.5146 & -0.6809 & -1.5162 \\
0.1523 & 0.2746 & 2.5530 & 0.2145 & 0.2834 & -0.2314 & 0.4514 \\
0.4130 & 0.2618 & -0.0231 & 0.3171 & 0.3507 & 0.7663 & -2.4392 \\
0.3739 & -0.0544 & 1.0088 & 0.0938 & 2.4110 & 0.1224 & -0.0533 \\
-2.5165 & 0.4874 & -0.2568 & -0.4748 & -0.1762 & 0.2814 & -0.1679 \\
-1.1412 & -0.2480 & 0.2974 & 0.2892 & 0.7346 & 1.3026 & 1.7966 \\
\end{bmatrix}
$$

The value of $Tr(\hat{M}_{22}(\xi_{A,s},7))$ is $1.8347$ and the radius is also close to $\sqrt{7}$.

Here we find that $A$- and $A_s$-optimal minimal-point designs for $k = 7$ are similar to each other from the table given below.

<table>
<thead>
<tr>
<th>$\xi_{A,7}$</th>
<th>$Tr(X^\top(\xi)X(\xi))^{-1}$</th>
<th>$Tr(\hat{M}_{22}(\xi))$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\xi_{A,7}$</td>
<td>3.3109</td>
<td>1.8660</td>
</tr>
<tr>
<td>$\xi_{A_s,7}$</td>
<td>3.3976</td>
<td>1.8347</td>
</tr>
</tbody>
</table>

### 3.2 Slope-rotatable minimal-point composite designs

Slope-rotatability has been studied in Hader and Park (1978), Park (1987), and Park and Kim (1992). They consider design aspects of response surface experiments in which emphasis is on estimation of differences in response rather than absolute value of the response variable. Estimation of differences in response at different points in the factor space will often be of great importance. If differences at points close together in the factor
space are involved, estimation of the local slopes (the rates of change) of the response surface is of interest.

In this thesis, a measure of slope-rotatability for response surface designs, proposed by Park and Kim (1992), is used. Define

\[ v_i = \text{Var}(\hat{\beta}_i), \quad v_{ii} = \text{Var}(\hat{\beta}_{ii}), \quad v_{ij} = \text{Var}(\hat{\beta}_{ij}), \]

\[ c_{i,ii} = \text{Cov}(\hat{\beta}_i, \hat{\beta}_{ii}), \quad c_{i,ij} = \text{Cov}(\hat{\beta}_i, \hat{\beta}_{ij}), \quad c_{ii,ij} = \text{Cov}(\hat{\beta}_{ii}, \hat{\beta}_{ij}), \quad c_{ij,il} = \text{Cov}(\hat{\beta}_{ij}, \hat{\beta}_{il}). \]

The measure of slope-rotatability, \( Q_k(\xi) \), is

\[ Q_k(\xi) = \frac{1}{2(k-1)^2} \left[ (k+2)(k+4)A_k + 2(k+4)B_k + 3C_k \right], \]

where

\[ A_k = \sum_{i=1}^{k} v_i^2 - \frac{1}{k} \left( \sum_{i=1}^{k} v_i \right)^2, \]

\[ B_k = \sum_{i=1}^{k} v_i (4v_{ii} + \sum_{j=1, j\neq i}^{k} v_{ij}) - \frac{1}{k} \left( \sum_{i=1}^{k} v_i \right)^2 \left( \sum_{j=1, j\neq i}^{k} (4v_{ii} + \sum_{j}^{k} v_{ij}) \right) + 2 \sum_{i=1}^{k} (4c_{i,ii}^2 + \sum_{j=1, j\neq i}^{k} c_{i,ij}^2), \]

\[ C_k = \sum_{i=1}^{k} (16v_{ii}^2 + \sum_{j=1, j\neq i}^{k} v_{ij}^2) - \frac{k+2}{3k} \left[ \sum_{i=1}^{k} (4v_{ii} + \sum_{j=1, j\neq i}^{k} v_{ij}) \right]^2 \]

\[ + \frac{2}{3} \sum_{i=1}^{k} (4v_{ii} \sum_{j=1, j\neq i}^{k} v_{ij} + \sum_{j=1, j\neq i}^{k} \sum_{j=1, j\neq i}^{k} v_{ij}v_{ii}) + \frac{4}{3} \sum_{i=1}^{k} (4 \sum_{j=1, j\neq i}^{k} c_{i,ii}^2 + \sum_{j=1, j\neq i}^{k} \sum_{j=1, j\neq i}^{k} c_{ij,il}^2). \]

Park and Kim (1992) showed that \( Q_k(\xi) \) is zero if and only if a design \( \xi \) is slope-rotatable, and \( Q_k(\xi) \) becomes larger as \( \xi \) deviates from a slope-rotatable design. Thus our objective function is set to be

\[ d_{Q,k}(r, \theta) = \frac{1}{2(k-1)^2} \left[ (k+2)(k+4)A_k + 2(k+4)B_k + 3C_k \right]. \]

In the following, for \( k = 2, 3, \ldots, 7 \), the minimal point composite designs for slope-rotatable criterion are shown.

### 3.2.1 Slope-rotatable minimal-point composite designs for \( k = 2 \)

For \( k = 2 \), the design space is the 2-ball with radius \( \sqrt{2} \) and one more point is added to form a minimal-point design. Then using polar coordinate representation in Equation (4), we have the following lemma for the measure of slope-rotatability.
Lemma 3. When $k = 2$, based on the $2^2$ factorial design, the measure of slope-rotatability is proportional to

$$Q_2(\xi) = \frac{1}{16} \left( 5 + \left( 960 \frac{r_1^4}{r_1^2} - 984 \frac{r_1^2}{r_1^4} \right) \sec[2\theta_{11}]^2 + \frac{4(16 - 6r_1^2 + 3r_1^4)^2}{r_1^8} \sec[2\theta_{11}]^4 \right).$$

It is easy to see that the minimum value of $Q_2(\xi)$ is obtained when $\theta_{11} = 0$. Since $Q_2(\xi)$ is a decreasing function with respect to $r_1$, the minimum value of $Q_2(\xi)$ is attended at $\theta_{11} = 0$ and $r_1 = \sqrt{2}$. Hence the added point is $(\sqrt{2}, 0)$, and at this time, the corresponding measure is 9.3281.

Now we use our BAR sampler to find the result numerically. With a random initial state, we suppose $T(t) = (5t)^{-2/3}$ and $N_t$ is set to be 10. Totally our algorithm is iterated 2500 times. The added point found by BAR sampler is

$$\left( 1.4142, 0.0000 \right).$$

This added point is very close to an axial point of the spherical CCD with two factors. In fact, the support point for slope-rotatable criterion is any one of four axial points. Figure 3 shows that the trend of the measure of slope-rotatability for the first 100 iterations, and from this figure, our algorithm quickly converges to a local extreme.

Figure 3: For $k=2$, the measure of slope-rotatable criterion for $10 \times 10 = 100$ steps.
3.2.2 Slope-rotatable minimal-point composite designs for $k = 3$

For $k = 3$, the first-order design is also chosen from the columns $(1, 2, 3)$ from 4-runs $P$-$B$ design. Five added points are required to form a minimal-point design. Since the measure of slope-rotatability is too difficult to write down its close form, we use the BAR sampler to find these five added points. We assume $T(t) = (5t)^{-2/3}$ and set $N_t = 10$. Totally our algorithm is iterated 2500 times, and the added points are

$$
\begin{bmatrix}
-0.5421 & -1.5554 & 0.5355 \\
0.5594 & 1.5501 & 0.5333 \\
-1.5524 & -0.5543 & 0.5319 \\
-0.0004 & -0.0074 & 1.7320 \\
1.5553 & 0.5468 & 0.5310 \\
\end{bmatrix}
$$

The measure of slope-rotatability is 0.7986, and the radiuses of those five added points are very close to $\sqrt{3}$. Hence, we conclude that these added points should be on the boundary of the design space $X$.

3.2.3 Slope-rotatable minimal-point composite designs for $k = 4$

For $k = 4$, there are 15 parameters in the second-order polynomial model, and the design space is the 4-ball with radius 2. The first-order design is $2^{4-1}$ fractional factorial design with resolution $III^*$. Therefore six added points are required for a minimal-point design. We apply our BAR sampler to find the minimum value of the measure of slope-rotatability with $T(t) = (20t)^{-2/3}$ and $N_t = 10$. After 2500 iterations, the added points we get are

$$
\begin{bmatrix}
-0.5820 & 1.8609 & -0.1304 & -0.4257 \\
1.5957 & 0.1715 & -1.0279 & -0.6064 \\
-1.8075 & 0.5422 & 0.4576 & -0.4791 \\
1.5934 & -1.0508 & 0.1563 & -0.5766 \\
-0.5627 & -0.1282 & 1.8645 & -0.4366 \\
0.1853 & 0.2272 & 0.2350 & 1.9644 \\
\end{bmatrix}
$$
The minimum value for measure of slope-rotatability is 0.5537. These six radii are very close to 2. However, if the initial angles are set to be

\[
\begin{bmatrix}
0 & \pi/2 & \pi/2 \\
\pi & \pi/2 & \pi/2 \\
\pi/2 & \pi/2 & \pi/2 \\
-\pi/2 & \pi/2 & \pi/2 \\
\pi/2 & 0 & \pi/2 \\
\pi/2 & \pi & \pi/2 
\end{bmatrix},
\]

then after 2500 iterations, these added points are

\[
\begin{bmatrix}
1.9989 & -0.0382 & 0.0421 & 0.0358 \\
-1.9964 & 0.0837 & 0.0704 & 0.0500 \\
-0.0098 & 1.9996 & 0.0020 & 0.0397 \\
0.1335 & -1.9870 & 0.0364 & -0.1804 \\
-0.0092 & -0.1274 & 1.9955 & 0.0397 \\
-0.0045 & 0.0505 & -1.9976 & 0.0838 
\end{bmatrix}.
\]

The measure of slope-rotatability is 0.3528.

Since these added points are close to axial points, we choose any six axial points to be our added points. We find that the measure of slope-rotatability is 0.3281 with \((\pm 2, 0, 0, 0), (0, \pm 2, 0, 0)\) and \((0, 0, \pm 2, 0)\). So the slope-rotatable minimal-point designs should be constructed by these axial points, \((\pm 2, 0, 0, 0), (0, \pm 2, 0, 0)\) and \((0, 0, \pm 2, 0)\).

### 3.2.4 Slope-rotatable minimal-point composite designs for \(k = 5\)

For \(k = 5\), two kind of first-order design are used. One is the \(2^{5-1}\) fractional factorial design with resolution \(V\) and the other is Plackett and Burman design for \(k = 5\).

#### \(2^{5-1}\) fractional factorial design with resolution \(V\)

When \(2^{5-1}\) fractional factorial design with resolution \(V\) is the first-order design, four added points are needed to form a minimal-point design. We use the BAR sampler to find the added points of slope-rotatable criterion with the assumptions, \(T(t) = (20t)^{-2/3}\)
and $N_t = 10$. After 2500 iterations, the minimum value of measure of slope-rotatability is 0.4893, and these added points are

$$
\begin{bmatrix}
0.0017 & -0.2146 & -0.2104 & -0.1727 & 2.2090 \\
0.0094 & 2.2202 & -0.1403 & -0.1796 & -0.1362 \\
-0.0024 & -0.2243 & 2.2104 & -0.1582 & -0.1974 \\
-0.0120 & -0.1664 & -0.1913 & 2.2157 & -0.1627 \\
\end{bmatrix}
$$

The radiuses of these four added points are close to $\sqrt{5}$, and these added support points are also close to axial points, $(0, 0, 0, 0, \sqrt{5})$, $(0, 0, \sqrt{5}, 0, 0)$, $(\sqrt{5}, 0, 0, 0, 0)$ and $(0, 0, 0, \sqrt{5}, 0)$. Then we replace the added points with these four axial points. However, the measure of slope-rotatability for four axial points is 0.5223. Thus, these axial points can not be our slope-rotatable added points.

**Plackett and Burman design for $k = 5$**

Now we discuss the case of Plackett and Burman design with $k = 5$. Here we need nine added points to form a minimal-point design. Applying our BAR sampler, we can find the added points of slope-rotatable criterion with the supposition, $T(t) = (20t)^{-2/3}$ and $N_t = 10$. Finally our algorithm is iterated 2500 times, and the added points that we find are

$$
\begin{bmatrix}
-0.1410 & -0.1375 & -0.1514 & -1.3968 & -1.7284 \\
0.2379 & 0.3102 & 0.2811 & 2.1643 & 0.2894 \\
-0.1330 & 2.1665 & -0.1782 & 0.5026 & -0.0664 \\
-1.7082 & -0.2093 & -0.1782 & -1.4086 & -0.1493 \\
-0.1477 & -0.1936 & 2.1768 & 0.4297 & -0.1321 \\
2.1728 & -0.1081 & -0.1504 & 0.4673 & -0.1618 \\
-0.0745 & -0.1697 & -1.7002 & -1.4327 & -0.1490 \\
-0.1226 & -1.7708 & -0.1073 & -1.3357 & -0.2317 \\
-0.1603 & -0.1349 & -0.1694 & 0.4414 & 2.1754 \\
\end{bmatrix}
$$

Hence the value of measure of slope-rotatability is 0.1043 and the radiuses of nine added points are also close to $\sqrt{5}$. 

27
3.2.5 Slope-rotatable minimal-point composite designs for $k = 6$

For $k = 6$, the $2^{6-2}$ factional factorial design with resolution $III^*$ is used as the first-order design. We need 11 added points to form our minimal-point design. However we can obtain that for $k = 2, 3, \ldots, 5$, the radiuses of those added points are all close to the boundary $\sqrt{k}$. Therefore we set all added points have the same radius $r$. Set $T(t) = (5t)^{-2/3}$ and $N_t = 10$ applying our BAR sampler, the added points after 1500 iterations, the added points we get are

$$
\begin{bmatrix}
0.2236 & -2.1978 & 0.6147 & -0.3311 & -0.5985 & -0.5233 \\
-0.8307 & 1.4405 & 1.0316 & -0.5066 & -1.2271 & -0.6390 \\
0.7508 & 1.1129 & -1.7356 & -0.6704 & -0.7233 & -0.4614 \\
-0.0226 & -0.0176 & 0.1143 & -0.3143 & -0.1550 & -2.4214 \\
-0.0371 & 0.0561 & -0.4046 & 1.2719 & 2.0509 & 0.0882 \\
0.3642 & -0.2658 & 0.2968 & -2.3573 & -0.3898 & -0.0066 \\
0.0167 & -0.0053 & 0.0093 & -0.0985 & 1.9939 & 1.4192 \\
0.6103 & -0.4132 & 2.2919 & -0.3282 & -0.3058 & -0.0536 \\
0.4532 & -0.0862 & 0.2479 & 0.9257 & -2.1712 & 0.3934 \\
2.3233 & -0.2373 & 0.0687 & -0.3281 & -0.4692 & -0.4621 \\
-1.4546 & -0.5803 & -1.4528 & -0.6589 & -0.9111 & -0.4156
\end{bmatrix}
$$

The numerically result is that the minimum value of measure of slope-rotatability is 0.0753 and the only radius is close to $\sqrt{6}$.

3.2.6 Slope-rotatable minimal-point composite designs for $k = 7$

For $k = 7$, the first-order design is the columns $(1, 2, 5, 6, 7, 9, 10)$ from 24-runs $P$-$B$ design without 3rd and 20th runs. We need 13 added points to form the minimal-point design and only one radius is used for these added points. We employ the BAR sampler to find the added points. Here we assume $T(t) = (20t)^{-2/3}$ and $N_t$ is set to be 10. Totally our algorithm is iterated 1500 times. The minimum value for measure of slope-rotatability
is 0.0461, and the only one radius is also close to $\sqrt{7}$. Hence those added points are

\[
\begin{bmatrix}
-0.4461 & 0.8086 & -0.3305 & 1.9853 & 1.3202 & 0.5038 & -0.3165 \\
-0.0865 & -0.5355 & -0.2649 & 0.8186 & -0.2674 & 0.6093 & 2.3501 \\
-2.3086 & -0.9999 & 0.0216 & 0.6002 & 0.4576 & 0.1931 & -0.2520 \\
-0.4478 & -0.4515 & -0.0139 & -0.2334 & -0.0692 & -2.4010 & -0.8784 \\
-0.2917 & -0.2231 & -0.6238 & 0.5307 & -0.4018 & -0.3968 & -2.4240 \\
2.0726 & 0.7764 & -0.0410 & -0.9695 & 0.2997 & 0.5561 & -0.8724 \\
0.2923 & -0.4255 & 0.4685 & -0.2340 & -2.5232 & 0.0315 & 0.3036 \\
0.6268 & 0.3692 & 0.1470 & -2.4476 & -0.5315 & -0.4162 & 0.0542 \\
-0.3907 & -2.2160 & 0.3648 & 0.9727 & -0.5667 & -0.6960 & -0.2286 \\
-0.0418 & 2.5191 & 0.4167 & -0.0572 & -0.5319 & -0.1303 & -0.4192 \\
0.1460 & 0.0335 & -2.6017 & 0.1696 & 0.1925 & 0.3781 & 0.0209 \\
-0.4434 & -0.7581 & -0.4401 & 0.4204 & -0.0479 & 2.3849 & 0.4103 \\
0.4374 & -1.0251 & 2.2089 & -0.5518 & -0.6220 & -0.1970 & -0.3857
\end{bmatrix}
\]

4 Comparison

In the last section, the minimal-point designs for three criteria are found numerically. Here first minimal-point designs for different criteria are compared to each other, and the relative efficiencies are used for comparisons among our designs and other minimal-point (and small composite) designs. For convenience, we denote $\xi_{Q_{k,k}}$ to be the minimal-point design for $k$ factors found by slope-rotatable criterion. In order to compare designs, we use optimal relative efficiency. Based on $\phi$-criterion, the $\phi$ relative efficiency of design $\xi_i$ relative to $\xi_\tau$ is defined as

$$\phi(\xi_i, \xi_\tau) = \frac{\phi(M(\xi_i))}{\phi(M(\xi_\tau))}.$$  

If this value is close to 1, these two designs are about equally informative in terms of the $\phi$-criterion. If $\phi(M(\xi_i))$ is larger than $\phi(M(\xi_\tau))$, then $\xi_\tau$ contains more information than $\xi_i$ in terms of the $\phi$-criterion.

From our numerical results in Section 3, $A$- and $A_s$-optimal minimal-point designs
First-order design $k$ $p$ design $\xi$ $Tr(X^\top(\xi)X(\xi))^{-1}$ $Q_k(\xi)$

$2^k$ fractional factorial designs with resolution $V$

<table>
<thead>
<tr>
<th>$k$</th>
<th>$p$</th>
<th>$\xi_{A,k}$</th>
<th>$\xi_{Q,k}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>6</td>
<td>3.2500</td>
<td>9.3281</td>
</tr>
<tr>
<td>5</td>
<td>21</td>
<td>2.6142</td>
<td>0.4976</td>
</tr>
</tbody>
</table>

$2^k$ fractional factorial designs with resolution $III^*$

<table>
<thead>
<tr>
<th>$k$</th>
<th>$p$</th>
<th>$\xi_{A,k}$</th>
<th>$\xi_{Q,k}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>15</td>
<td>2.8612</td>
<td>1.1027</td>
</tr>
<tr>
<td>6</td>
<td>28</td>
<td>2.5721</td>
<td>0.4957</td>
</tr>
</tbody>
</table>

$P$-$B$ designs

<table>
<thead>
<tr>
<th>$k$</th>
<th>$p$</th>
<th>$\xi_{A,k}$</th>
<th>$\xi_{Q,k}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>10</td>
<td>2.8788</td>
<td>0.9694</td>
</tr>
<tr>
<td>5</td>
<td>21</td>
<td>2.6461</td>
<td>0.4388</td>
</tr>
<tr>
<td>7</td>
<td>36</td>
<td>3.3109</td>
<td>0.1193</td>
</tr>
</tbody>
</table>

Table 2: Compare our $A$-optimal and slope-rotatable minimal-point designs.

should be similar to each other. Therefore, here we only compare $A$-optimal and slope-rotatable minimal-point designs here. The $Tr(X^\top(\xi)X(\xi))^{-1}$ of slope-rotatable minimal-point designs and the values of $Q_k(\xi)$ of $A$-optimal minimal-point designs are shown in Table 2. From this table, we observe that when the first-order design is $2^k$ fractional factorial designs with resolution $V$, the $A$-optimal and slope-rotatable minimal-point designs are similar to each other, because the relative efficiencies, shown in Table 3, are 1, 0.9977 ($A$-optimal criterion) and 1, 0.9833 ($Q_k$ criterion). In fact, from Lemmas 1 and 3, when $k = 2$, these two minimal-point designs are the same. From Table 3, the relative efficiencies $A(\xi_{Q,k}, \xi_A)$ are all at least 80%. Hence the slope-rotatable minimal-point designs are contain at least 80% information of $A$-optimal minimal-point designs. However, except $k = 3$, the $Q_k$ relative efficiencies of $\xi_A$ relative to $\xi_{Q,k}$ are less than 0.5.
Thus it seems that slope-rotatable minimal-point design is a robust designs among the $A$, $A_s$-optimal and slope-rotatable criteria.

Before we compare our designs with other minimal-point and small composite designs, we have some notations. We define $\xi_{CCD}$ is the spherical CCD with $n_{CCD}$ supports. The small composite designs proposed by Draper and Lin (1990) are denoted as $\xi_{small}$ with $n_{small}$ support points. Since the small composite designs still have more than $p$ support points, the two types of minimal-point designs also are constructed here by choosing $p - n_1 - 1$ axial points according to $A$-optimal and $Q_k$ criteria. Here these two types of designs are denoted by $\xi_{min,A}$ and $\xi_{min,Q_k}$. Hence we have Table 4 to show the differ-

<table>
<thead>
<tr>
<th>First-order design</th>
<th>$k$</th>
<th>$p$</th>
<th>$A(\xi_{Q_k}, \xi_A)$</th>
<th>$Q_k(\xi_A, \xi_{Q_k})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2^k$ fractional factorial designs with resolution $V$</td>
<td>2</td>
<td>6</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>21</td>
<td>0.9977</td>
<td>0.9833</td>
</tr>
<tr>
<td>$2^k$ fractional factorial designs with resolution $III^*$</td>
<td>4</td>
<td>15</td>
<td>0.8976</td>
<td>0.2975</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>28</td>
<td>0.8884</td>
<td>0.1638</td>
</tr>
<tr>
<td>$P-B$ designs</td>
<td>3</td>
<td>10</td>
<td>0.9596</td>
<td>0.8238</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>21</td>
<td>0.7996</td>
<td>0.2377</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>36</td>
<td>0.8639</td>
<td>0.3864</td>
</tr>
</tbody>
</table>

Table 3: The relative efficiencies between $A$-optimal and slope-rotatable minimal-point designs.

<table>
<thead>
<tr>
<th>$k$</th>
<th>$p$</th>
<th>$n_{CCD}$</th>
<th>$n_{small}$</th>
<th>$n_C$</th>
<th>$n_{min}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>6</td>
<td>9</td>
<td>ND</td>
<td>7</td>
<td>6</td>
</tr>
<tr>
<td>3</td>
<td>10</td>
<td>15</td>
<td>11</td>
<td>11</td>
<td>10</td>
</tr>
<tr>
<td>4</td>
<td>15</td>
<td>25</td>
<td>17</td>
<td>16</td>
<td>15</td>
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<td>5</td>
<td>21</td>
<td>27</td>
<td>22</td>
<td>22</td>
<td>21</td>
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<tr>
<td>6</td>
<td>28</td>
<td>45</td>
<td>29</td>
<td>29</td>
<td>28</td>
</tr>
<tr>
<td>7</td>
<td>36</td>
<td>79</td>
<td>37</td>
<td>37</td>
<td>36</td>
</tr>
</tbody>
</table>

Table 4: The number of supports in CCDs, small composite designs and minimal-point designs.
ent numbers of design points for $\xi_{\text{CCD}}$, $\xi_{\text{small}}$, and $\xi_{\text{min}}$. Next, we compare our designs with other minimal-point and small composite designs according to two different criteria, $A$-optimal and $Q_k$ criteria.

**Comparison according to $A$-optimal criterion**

In this part, we would compare our $A$-optimal minimal-point designs with spherical CCDs and other small composite designs. To fairly compare designs, we use the relative $A$-optimal point efficiencies, which are defined as

$$A\text{-Peff}(\xi_{\text{CCD}}, \xi_A) = \frac{n_A}{n_{\text{CCD}}} A(\xi_{\text{CCD}}, \xi_A);$$

$$A\text{-Peff}(\xi_{\text{small}}, \xi_A) = \frac{n_A}{n_{\text{small}}} A(\xi_{\text{small}}, \xi_A);$$

$$A\text{-Peff}(\xi_{\text{min}}, \xi_A) = A(\xi_{\text{min}}, \xi_A).$$

When the relative $A$-optimal point efficiency is less than 1, our $A$-optimal minimal-point design is better. The values of the trace of $(X^\top X)^{-1}$ and the relative $A$-optimal point efficiencies are displayed in Table 5 and 6. From Table 5, our $A$-optimal minimal-point designs are better than the CCD’s, because all values of $A\text{-Peff}$ are less than 1.

When we compare with other small composite designs and minimal-point designs, except the cases that the first-order designs are resolution $V$ designs, our $A$-optimal minimal-point designs are always better than other designs significantly. For $k = 2$ and 5 and

<table>
<thead>
<tr>
<th>$k$</th>
<th>$p$</th>
<th>$\xi_{\text{CCD}}$</th>
<th>$\xi_A$</th>
<th>$A\text{-Peff}(\xi_{\text{CCD}}, \xi_A)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>6</td>
<td>2.1875</td>
<td>$V$</td>
<td>3.2500</td>
</tr>
<tr>
<td>3</td>
<td>10</td>
<td>2.0575</td>
<td>$P-B$</td>
<td>2.8788</td>
</tr>
<tr>
<td>4</td>
<td>15</td>
<td>1.8958</td>
<td>$III^*$</td>
<td>2.8612</td>
</tr>
<tr>
<td>5</td>
<td>21</td>
<td>2.1050</td>
<td>$V$</td>
<td>2.6142</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$P-B$</td>
<td>2.8788</td>
</tr>
<tr>
<td>6</td>
<td>28</td>
<td>1.8450</td>
<td>$III^*$</td>
<td>2.5721</td>
</tr>
<tr>
<td>7</td>
<td>36</td>
<td>1.6238</td>
<td>$P-B$</td>
<td>3.3109</td>
</tr>
</tbody>
</table>

Table 5: The trace of $(X^\top X)^{-1}$ and relative $A$-optimal point efficiencies of $\xi_{\text{CCD}}$ and $\xi_A$. 

32
\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
k & p & \xi_{small} & \xi_{min,A} & \xi_A & A\text{-Peff}(\xi_{small}, \xi_A) & A\text{-Peff}(\xi_{min,A}, \xi_A) \\
\hline
V & 2 & 6 & ND & 3.2500 & 3.2500 & ND & 1 \\
 & 5 & 21 & ND & 2.6200 & 2.6142 & ND & 0.9978 \\
III* & 4 & 15 & 2.9219 & 3.1875 & 2.8612 & 0.8640 & 0.8976 \\
 & 6 & 28 & 3.1796 & 5.0556 & 2.5721 & 0.7810 & 0.5088 \\
P-B & 3 & 10 & 3.2278 & 6.0556 & 2.8788 & 0.8108 & 0.4754 \\
 & 5 & 21 & 4.4263 & 8.0164 & 2.6461 & 0.5706 & 0.3300 \\
 & 7 & 36 & 21.6870 & 26.1207 & 3.3109 & 0.1485 & 0.1268 \\
\hline
\end{array}
\]
Table 6: The trace of \((X^\top X)^{-1}\) and relative \(A\)-optimal point efficiencies of \(\xi_{small}, \xi_{min}\) and \(\xi_A\).

\[
\begin{array}{|c|c|c|c|c|}
\hline
k & p & \xi_{CCD} & \xi_{Q_k} & Q_k(\xi_{CCD}, \xi_{Q_k}) \\
\hline
2 & 6 & 1.2656 & V & 9.3281 & 7.3705 \\
3 & 10 & 0.2496 & P-B & 0.7986 & 3.2034 \\
4 & 15 & 0.0851 & III* & 0.3281 & 3.8554 \\
5 & 21 & 0.0281 & V & 0.4893 & 17.4128 \\
 & & & P-B & 0.1043 & 3.7117 \\
6 & 28 & 0.0166 & III* & 0.0753 & 1.5361 \\
7 & 36 & 0.0103 & P-B & 0.0461 & 4.4757 \\
\hline
\end{array}
\]
Table 7: The measure of \(Q_k(\xi)\) and relative efficiencies of \(\xi_{CCD}\) and \(\xi_{Q_k}\).

resolution \(V\) designs as the first-order designs, these two types of minimal-point designs should be similar to each other because \(A\)-Peff are equal to 1 and 0.9978.

Comparison according to slope-rotatable criterion

Now the slope-rotatable criterion is considered. Park and Kim (1992) showed that \(Q_k\) is invariant with respect to the scaling constant. The values of \(Q_k\) and relative \(Q_k\)-efficiencies are displayed in Table 7 and 8. From these tables, we can observe that:

- Central composite designs vs. slope-rotatable minimal-point designs:

  From Table 7, spherical CCDs all provide the better information than on slope-
rotatable minimal-point designs in terms of $Q_k$ criterion. But for large $k$, $k = 6$ and 7, CCD’s and our minimal-point designs should close to slope-rotatable, because the values of $Q_k$ are close to 0.

- **Small composite designs vs. slope-rotatable minimal-point designs:**
  For $k = 3$ and 4, $\xi_{small}$ have better performances than our slope-rotatable minimal-point designs. But for $k = 5$ and 7, our minimal-point designs are better than $\xi_{small}$. Finally for $k = 6$, the values of $Q_k$ for both designs are close to 0.

- **Other minimal-point designs vs. slope-rotatable minimal-point designs:**
  When the first-order design is $2^k$ fractional factorial design with resolution $V$, our slope-rotatable minimal-point designs have similar performances with $\xi_{min,Q_k}$. This is because the added support points of our slope-rotatable minimal-point designs for $2^k$ fractional factorial designs with resolution $V$ are close to axial points. When $P-B$ designs are the first-order designs, our slope-rotatable minimal-point designs have better performances than these of minimal-point designs in terms of $Q_k$ criterion, except the case of $k = 4$. It may due to $P-B$ designs do not have symmetric structure in the design space.
5 Conclusion

In this thesis, the minimal-point second-order designs are constructed according to three different criteria on the spherical design space. Since design space is the ball, the spherical coordinate is used here to represent the experimental points. Here our problem is transformed as the optimization problems. When the objective function is too complicate to optimize directly, a simulated annealing type algorithm, the Best Angles and Radius Sampler, is used for finding the added support points. In Section 4, we compare our minimal-point designs with other designs, included CCD’s, small composite designs, and some minimal-point designs for different criteria, $A$-optimal and slope-rotatable criteria.

Here we have the following conclusions:

1. No matter what criterion is used, these added points should be on the boundary of the $k$-ball with radius $\sqrt{k}$.

2. $A$- and $A_s$-optimal minimal-point designs should be similar to each other.

3. For $A$-optimal and slope-rotatable criteria, slope-rotatable minimal-point designs are more robust.

4. Based on $A$-optimal criterion, our $A$-optimal minimal-point designs are always better then CCD’s, $\xi_{small}$ and $\xi_{min,A}$.

5. In terms of slope-rotatability, CCD’s have the best performance among all four types of designs. For large $k$, the values of $Q_k$ of our slope-rotatable minimal-point designs are also close to 0. From our comparisons, it seems that the more design points are, the lower $Q_k$ is.

In this thesis, the added points are selected according to a given criterion. However, for each $k$, the number of the possible first-order designs might be more than 1. Thus one of future work would be that we also need to choose the first-order designs according to a criterion. Then we believe this kind of minimal-point designs should have better performance.
Appendix:

The Figures of $A$- and $A_s$-optimal and Slope-rotatable Criteria

A.1 $A$-optimal minimal-point composite designs
A.2 $A_s$-optimal minimal-point composite designs
A.3 Slope-rotatability minimal-point composite designs
A.1 $A$-optimal minimal-point composite designs

Figure 4: For $k = 3$, the radiuses of $A$-optimal criterion for $2500 \times 10 = 25000$ steps.

Figure 5: For $k = 3$, the trace of $A$-optimal criterion for $2500 \times 10 = 25000$ steps.

Figure 6: For $k = 4$, the radiuses of $A$-optimal criterion for $2500 \times 10 = 25000$ steps.

Figure 7: For $k = 4$, the trace of $A$-optimal criterion for $2500 \times 10 = 25000$ steps.
Figure 8: For $2^{5-1}$ fractional factorial with resolution V, the radiuses of A-optimal criterion for $2500 \times 10 = 25000$ steps.

Figure 9: For $2^{5-1}$ fractional factorial with resolution V, the trace of A-optimal criterion for $2500 \times 10 = 25000$ steps.

Figure 10: For $P-B$ design with $k = 5$, the radiuses of A-optimal criterion for $2500 \times 10 = 25000$ steps.

Figure 11: For $P-B$ design with $k = 5$, the trace of A-optimal criterion for $2500 \times 10 = 25000$ steps.
Figure 12: For $k = 6$, the radiuses of $A$-optimal criterion for $1500 \times 10 = 15000$ steps.

Figure 13: For $k = 6$, the trace of $A$-optimal criterion for $1500 \times 10 = 15000$ steps.

Figure 14: For $k = 7$, the radiuses of $A$-optimal criterion for $1500 \times 10 = 15000$ steps.

Figure 15: For $k = 7$, the trace of $A$-optimal criterion for $1500 \times 10 = 15000$ steps.
A.2  $A_s$-optimal minimal-point composite designs

Figure 16: For $k = 3$, the radiuses of $A_s$-optimal criterion for $2500 \times 10 = 25000$ steps.

Figure 17: For $k = 3$, the trace of $A_s$-optimal criterion for $2500 \times 10 = 25000$ steps.

Figure 18: For $k = 4$, the radiuses of $A_s$-optimal criterion for $2500 \times 10 = 25000$ steps.

Figure 19: For $k = 4$, the trace of $A_s$-optimal criterion for $2500 \times 10 = 25000$ steps.
Figure 20: For $2^{5-1}$ fractional factorial with resolution $V$, the radiuses of $A_s$-optimal criterion for $2500 \times 10 = 25000$ steps.

Figure 21: For $2^{5-1}$ fractional factorial with resolution $V$, the trace of $A_s$-optimal criterion for $2500 \times 10 = 25000$ steps.

Figure 22: For $P-B$ design with $k = 5$, the radiuses of $A_s$-optimal criterion for $2500 \times 10 = 25000$ steps.

Figure 23: For $P-B$ design with $k = 5$, the trace of $A_s$-optimal criterion for $2500 \times 10 = 25000$ steps.
Figure 24: For $k = 6$, the radiuses of $A_s$-optimal criterion for $1500 \times 10 = 15000$ steps.

Figure 25: For $k = 6$, the trace of $A_s$-optimal criterion for $1500 \times 10 = 15000$ steps.

Figure 26: For $k = 7$, the radiuses of $A_s$-optimal criterion for $1500 \times 10 = 15000$ steps.

Figure 27: For $k = 7$, the trace of $A_s$-optimal criterion for $1500 \times 10 = 15000$ steps.
A.3 slope-rotatability minimal-point composite designs

Figure 28: For $k = 3$, the radiuses of slope-rotatable criterion for $2500 \times 10 = 25000$ steps.

Figure 29: For $k = 3$, the measure of slope-rotatable criterion for $2500 \times 10 = 25000$ steps.

Figure 30: For $k = 4$, the radiuses of slope-rotatable criterion for $2500 \times 10 = 25000$ steps.

Figure 31: For $k = 4$, the measure of slope-rotatable criterion for $2500 \times 10 = 25000$ steps.
Figure 32: For $2^{5-1}$ fractional factorial with resolution $V$, the radiuses of slope-rotatable criterion for $2500 \times 10 = 25000$ steps.

Figure 33: For $2^{5-1}$ fractional factorial with resolution $V$, the measure of slope-rotatable criterion for $2500 \times 10 = 25000$ steps.

Figure 34: For $P-B$ design with $k = 5$, the radiuses of slope-rotatable criterion for $2500 \times 10 = 25000$ steps.

Figure 35: For $P-B$ design with $k = 5$, the measure of slope-rotatable criterion for $2500 \times 10 = 25000$ steps.
Figure 36: For $k = 6$, the radiiuses of slope-rotatable criterion for $1500 \times 10 = 15000$ steps.

Figure 37: For $k = 6$, the measure of slope-rotatable criterion for $1500 \times 10 = 15000$ steps.

Figure 38: For $k = 7$, the radiiuses of slope-rotatable criterion for $1500 \times 10 = 15000$ steps.

Figure 39: For $k = 7$, the measure of slope-rotatable criterion for $1500 \times 10 = 15000$ steps.
References


