# A-optimal Minimax Design Criterion for

# Two-level Fractional Factorial Designs

by

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BA. Beijing Institute of Technology 2011

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# Abstract

In this thesis we introduce and study an A-optimal minimax design criterion for two-level fractional factorial designs, which can be used to estimate a linear model with main effects and some interactions. The resulting designs are called A-optimal minimax designs, and they are robust against the misspecification of the terms in the linear model. They are also efficient, and often they are the same as A-optimal and D-optimal designs. Various theoretical results about A-optimal minimax designs are derived. A couple of search algorithms including a simulated annealing algorithm are discussed to search for optimal designs, and many interesting examples are presented in the thesis.

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# Chapter 1

# Introduction

Experimental designs are important and useful to study the performance of processes and systems. There are applications in many research areas such as quality control in industry, maximizing crop yield in agriculture, marketing research in business, and developing new drugs in medicine. Various designs have been investigated in the literature, including factorial designs (Montgomery, 2006; Mukerjee and Wu, 2006), optimal regression designs (Pukelsheim, 1993), robust minimax regression designs (Huber, 1981; Wiens, 1992), and robust parameter designs (Montgomery, 2006). In this thesis, we introduce a minimax design criterion for two-level fractional factorial designs and study its properties.

Chapter 1 is organized as follows. Section 1.1 gives an overview of experimental designs while Section 1.2 briefly introduces factorial and fractional factorial designs. Section 1.3 contains the research problem of this thesis. Section 1.4 highlights the main contributions in this thesis.

## 1.1 Experimental design

Experimental design and analysis have been studied for a long time as a result of many benefits from optimal designs. A good design can help improve process yields as well as reduce variability, development time and overall costs (Montgomery, 2006). Three basic principles for a good design are randomization, replication and blocking (Montgomery, 2006). Randomization refers to that both the order of runs and the

allocation of experimental materials are to be performed randomly, which provide an access to get independent errors. Replication is to run independent repeat of each factor combination and it is used to reduce the variance of estimators. Blocking is a design technique to reduce variability from nuisance factors and improve the precision.

Considering the two major aspects of experimental design, the design of the experiment and the statistical analysis of the data (Montgomery, 2006), an investigator can construct different types of designs to match the requirements and draw meaningful conclusions. A design of experiment with only one factor to be investigated can be studied by one-way analysis of variance (ANOVA). In industry, if an engineer is willing to test how one factor with different levels (treatments) affects the response, one-way ANOVA can be used with hypothesis of no difference in levels. Randomized complete block design (RCBD) and Latin squares design are applied when an engineer studies one influential factor with possible nuisance factors. Randomization is used to reduce the effect of nuisance factors which are uncontrollable while blocking is used for controllable nuisance factors. A RCBD is used to block one nuisance factor and a Latin squares design is used to block two nuisance factors. For example, a RCBD with 4 levels in 4 blocks is given in Figure 1.1, where each column stands for one block, and A, B, C and D denote the 4 treatments.. Within each block, there is a complete replicate of the 4 treatments and the run order is randomized. In the situation of two nuisance factors, a Latin squares design can be applied and Figure 1.2 shows one Latin squares design with 4 treatments.

## 1.2   Factorial and fractional factorial designs

Factorial designs are useful to study two or more factors in an experiment. In this thesis, we will focus on two-level factorial designs, where all the factors take two levels. The total number of runs is $N = 2 \times 2 \times \cdots \times 2 = 2^k$ if there are $k$ factors. Statistical

Block

|   1   |   2   |   3   |   4   |
|-------|-------|-------|-------|
|   C   |   C   |   B   |   A   |
|   A   |   D   |   A   |   D   |
|   D   |   B   |   C   |   B   |
|   B   |   A   |   D   |   C   |

Figure 1.1: RCBD with 4 treatments (A, B, C, D) in 4 blocks.

Column nuisance factor

|                      |   | 1 | 2 | 3 | 4 |
|----------------------|---|---|---|---|---|
|                      | 1 | A | B | C | D |
| Row nuisance factor  | 2 | B | C | D | A |
|                      | 3 | C | D | A | B |
|                      | 4 | D | A | B | C |

Figure 1.2: Latin squares design with 4 treatments (A, B, C, D).

analysis can be performed by building specific models to estimate the effects. Both the effect model and linear regression model can be used to study factorial designs. Usually a full model with all the main effects and interaction terms is used for a full factorial design. In practice, restricted by the expensive spending, an engineer may need to construct fractional factorial designs with some specific combinations among all the runs. If some effects are known to be significant, a reduced model with only significant terms can be used to estimate the effects generated from fractional factorial designs.

Chapter 2 will review more details of factorial designs, and some examples and analysis based on reduced linear regression models are presented.

## 1.3   Research problems

Two-level fractional factorial designs are widely applied in many fields. How to construct a two-level fractional factorial design becomes an important issue for engineers. Wilmut and Zhou (2011) introduced one new method called D-optimal minimax design criterion for constructing the designs. This criterion is to minimize the largest determinant of the mean squared error of the least squares estimator. Motivated by the idea of D-optimal minimax design criterion, we consider a similar criterion, A-optimal minimax design criterion, for choosing the optimal designs. In addition, optimal designs from various optimal criteria are computed and compared.

The organization of the thesis is as follows. In Chapter 2, we review the factorial and fractional factorial designs with some examples. In Chapter 3, some existing design criteria are reviewed, and the A-optimal minimax design criterion is proposed. Several theoretical results are derived for A-optimal minimax designs. In Chapter 4, we discuss two algorithms to search for optimal designs. Many examples of A-optimal minimax designs are given and the designs are compared with A-optimal, D-optimal

and D-optimal minimax designs. Conclusion is given in Chapter 5.

## 1.4 Main contributions

The thesis contains the following main contributions:

(1) An A-optimal minimax design criterion is proposed and explored for fractional factorial designs.

(2) Various theoretical properties for A-optimal minimax designs are derived and illustrated by examples.

(3) An annealing algorithm is discussed and is effective to search for optimal designs.

(4) Many numerical results are presented for A-optimal minimax designs. New optimal designs are obtained for some linear models.

# Chapter 2

# Factorial design

In this chapter, we briefly review the design and analysis of factorial designs. In a factorial design with $k$ factors, we use $F_1$, $F_2$, ..., $F_k$ to denote the factors and use $y$ for a response variable. Suppose there are $a_i$ levels for factor $F_i$, and a full factorial design has $N = a_1 a_2 \cdots a_k$ runs. Using a full factorial design, we can estimate all the main effects, $F_1$, $F_2$, ..., $F_k$, and all the interactions among the factors. An $s$-factor $(2 \leq s \leq k)$ interaction is denoted by $F_{i_1} F_{i_2} \cdots F_{i_s}$, where $\{i_1, \cdots, i_s\}$ is a subset of $\{1, 2, \cdots, k\}$. In Section 2.1, two examples are presented to illustrate the notation of main effects and interactions, linear models, and regression analysis. In Section 2.2, we discuss some properties of the full and reduced linear models and introduce a requirement set for factorial designs.

## 2.1    Examples

**Example 2.1.** Suppose an engineer wants to design a battery for a device which will be used in various conditions in temperature (Montgomery, 2006). What he knows is that both the temperature and type of materials will affect the life of battery, but he doesn't know exactly how the temperature and material type influence the life. A test for battery with three different types of materials and three different conditions in temperature is run by the engineer to answer the following questions. What effect does temperature have on the life? Which type of materials is the best for three conditions in temperature compared with the other two types? A full factorial design

with 4 replicates is used for the test, and the results for the test are from Montgomery (2006) and are presented in Table 2.1.

Table 2.1: Life (in hours) data for the battery design example

| Material | Temperature (°F) | | | | | |
|---|---|---|---|---|---|---|
| Type | 15 | | 70 | | 125 | |
| 1 | 130 | 155 | 34 | 40 | 20 | 70 |
| | 74 | 180 | 80 | 75 | 82 | 58 |
| 2 | 150 | 188 | 136 | 122 | 25 | 70 |
| | 159 | 126 | 106 | 115 | 58 | 45 |
| 3 | 138 | 110 | 174 | 120 | 96 | 104 |
| | 168 | 160 | 150 | 139 | 82 | 60 |

Here, the two factors are material type ($F_1$) and temperature ($F_2$). The interaction between $F_1$ and $F_2$ is denoted by $F_1F_2$. Figure 2.1 shows four plots, which help us analyze the data: (a) 9 combinations for the two factors, (b) box-plot of the life data versus material type, (c) box-plot of the life data versus temperature, (d) an interaction plot between material type and temperature. Material type 3 seems to be the best one among all the three types of materials since the expected life is the longest. Low temperature seems to be excellent condition for long life. For all the three types, as the temperature goes up, the life of battery decreases. This implies that the longer life can be reached at the lower temperature. When the temperature changes from 15 °F to 70 °F, battery life for both material types 1 and 2 decreases. Especially, the life time of type 1 goes down dramatically while the life time of type 3 seems unchanged. When the temperature changes from 70 °F to 125 °F, the battery life seems unchanged for type 1, whereas for types 2 and 3 it decreased. Material
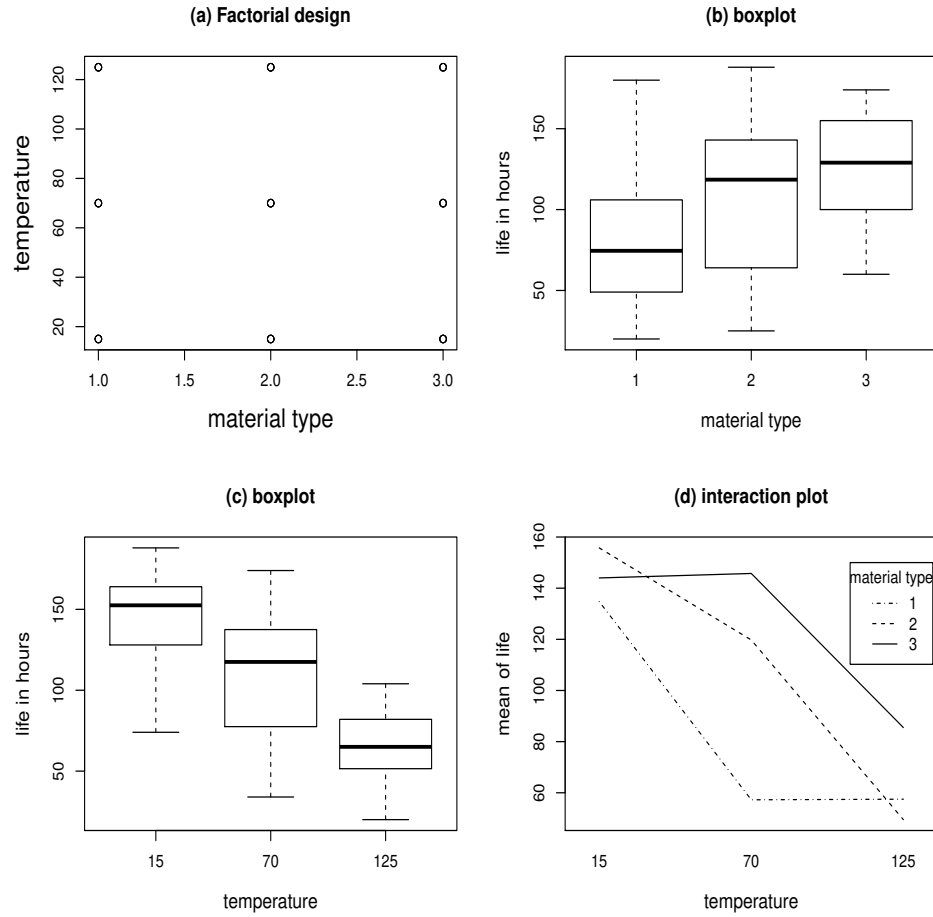
Figure 2.1: Plots for Example 2.1: (a) 9 combinations for the two factors, (b) box-plot of the life data versus material type, (c) box-plot of the life data versus temperature, (d) an interaction plot between material type and temperature.

type 3 seems to be the best choice.

Table 2.2: Regression variables

| Factor levels | | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1x_3$ | $x_2x_3$ | $x_1x_4$ | $x_2x_4$ |
|---|---|---|---|---|---|---|---|---|---|
| $F_1$ | $F_2$ | | | | | | | | |
| 1 | 15 | −1 | 1 | −1 | 1 | 1 | −1 | −1 | 1 |
| 1 | 70 | −1 | 1 | 0 | −2 | 0 | 0 | 2 | −2 |
| 1 | 125 | −1 | 1 | 1 | 1 | −1 | 1 | −1 | 1 |
| 2 | 15 | 0 | −2 | −1 | 1 | 0 | 2 | 0 | −2 |
| 2 | 70 | 0 | −2 | 0 | −2 | 0 | 0 | 0 | 4 |
| 2 | 125 | 0 | −2 | 1 | 1 | 0 | −2 | 0 | −2 |
| 3 | 15 | 1 | 1 | −1 | 1 | −1 | −1 | 1 | 1 |
| 3 | 70 | 1 | 1 | 0 | −2 | 0 | 0 | −2 | −2 |
| 3 | 125 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |

The header row for the table spans "Factor levels" over the $F_1$, $F_2$ columns and "Regression variables" over the remaining columns.

Since both factors have 3 levels, there are 2 degrees of freedom for the main effect of each factor and 4 degrees of freedom for the 2-factor interaction. To analyze the data, we use a linear regression model as follows,

$$y_i = \theta_0 + x_{i1}\theta_1 + x_{i2}\theta_2 + x_{i3}\theta_3 + x_{i4}\theta_4 + x_{i1}x_{i3}\theta_5 + x_{i2}x_{i3}\theta_6 + x_{i1}x_{i4}\theta_7 + x_{i2}x_{i4}\theta_8 + \varepsilon_i, \quad (2.1)$$

where variables $x_1$, $x_2$, $x_3$ and $x_4$ are defined in Table 2.2, and $y_i$ is the observed response at the $i$th run. Variables $x_1$ and $x_2$ are for the linear and quadratic effects of factor $F_1$, variables $x_3$ and $x_4$ are for the linear and quadratic effects of factor $F_2$, and $x_1x_3, x_2x_3, x_1x_4$ and $x_2x_4$ represent the interaction between $F_1$ and $F_2$.

For the full factorial design, the regressors coded in Table 2.2 are orthogonal.

Using the least squares estimation method, we obtain the fitted model as

$$\hat{y} = 105.528_{(4.331)} + 20.958_{(5.304)}x_1 - 1.403_{(3.062)}x_2 - 40.333_{(5.304)}x_3 - 1.028_{(3.062)}x_4$$

$$+4.687_{(6.496)}x_1x_3 + 6.396_{(3.751)}x_2x_3 - 11.646_{(3.751)}x_1x_4 + 2.340_{(2.165)}x_2x_4, \quad (2.2)$$

where the numbers in the brackets are the standard errors.

The residuals are shown in Figure 2.2: (a) residual versus fitted value, (b) residual versus material type, (c) residual versus temperature, (d) normal Q-Q plot of residuals. From these plots, the error variance seems to be constant and there is no problem of the normality assumption of the errors. From the results in model (2.2), it is clear that $x_1$, $x_3$ and $x_1x_4$ are significant in the linear model. Thus both the main effects and interaction effect have significant influence on the response.

From model (2.2), the expected life for the three types of materials is given in Table 2.3, and type 3 maximize the total life at the three levels of temperature. □

Table 2.3: Estimated expected life in Example 2.1

| $F_1$ (material type) | 1 | 1 | 1 | 2 | 2 | 2 | 3 | 3 | 3 |
|---|---|---|---|---|---|---|---|---|---|
| $F_2$ (temperature) | 15 | 70 | 125 | 15 | 70 | 125 | 15 | 70 | 125 |
| Estimated expected life (hours) | 134.7 | 57.3 | 57.5 | 155.8 | 119.8 | 49.5 | 144.0 | 145.8 | 85.5 |

**Example 2.2.** A laboratory assistant wants to get uniform fill heights in the soft drink bottles, since there are deviations generated in practice compared to the correct target height (Montgomery, 2006). In this case, the assistant needs to examine what the effects the following three factors have on the deviation from the target fill height for soft drink bottles, percent carbonation, line speed and operating pressure in the
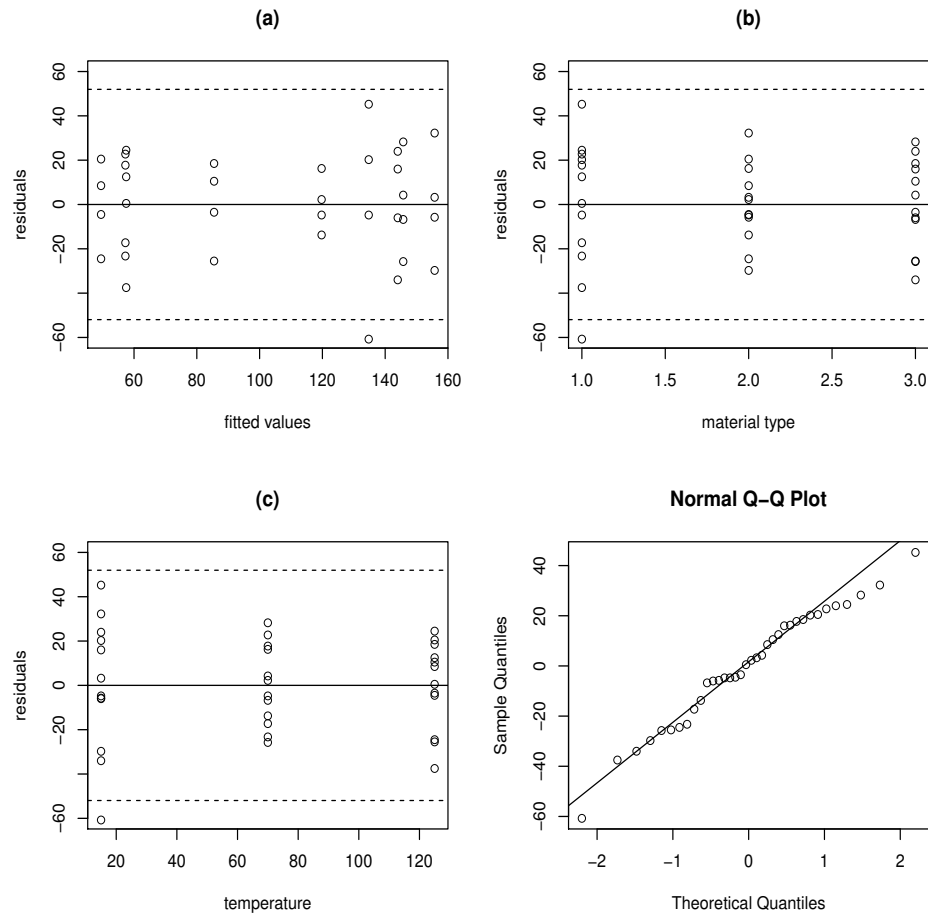
Figure 2.2: Residual plots for Example 2.1: (a) residual versus fitted value, (b) residual versus material type, (c) residual versus temperature, (d) normal Q-Q plot of residuals. The dotted horizontal lines in (a), (b) and (c) are $\pm 2\hat{\sigma}$, where $\hat{\sigma}$ is the estimated standard deviation of the errors.

filler which can be all controlled in practice. In this example, each factor takes two levels, and the total number of combinations is $N = 2 \times 2 \times 2 = 8$. The assistant chooses 10 percent and 12 percent as the two levels for percent carbonation, 200bpm (bottles per minute) and 250bpm as the two levels for line speed, and 25psi (pound per square inch) and 30psi as the two levels for operating pressure. A full factorial design with 2 replicates is used in this experiment and the results are shown in Table 2.4, where the response in this case is the difference between the actual value and the target value. Positive deviations are the heights above the target, while the negative deviations are the heights below the target.

Various plots of the data are constructed in Figure 2.3: (a) box-plot of deviation versus percent carbonation, (b) box-plot of deviation versus operating pressure, (c) box-plot of deviation versus line speed, (d) an interaction plot between percent and pressure, (e) an interaction plot between pressure and speed, and (f) an interaction plot between speed and percent. We notice that all three factors have positive effects for increasing the deviation from the target height. From the interaction plots (d), (e) and (f), all the interactions are probably small.

The three factors $F_1$, $F_2$ and $F_3$ denote percent carbonation, line speed and operating pressure, respectively. We use standard codes $+1$ and $-1$ to denote the two levels of a factor, and the interactions among the factors can be formed easily, which are presented in Table 2.5. Notice that all the effects are orthogonal for a full factorial design. Each main effect of a factor has 1 degree of freedom, and so is each interaction.

A full model including all the main effects and interactions for the three factors is fitted in software R, and the fitted model is,

$$
\begin{aligned}
\hat{y} &= 1.00_{(0.1976)} + 1.50_{(0.1976)}x_1 + 0.875_{(0.1976)}x_2 + 1.125_{(0.1976)}x_3 + 0.125_{(0.1976)}x_1x_2 \\
&\quad + 0.375_{(0.1976)}x_1x_3 + 0.25_{(0.1976)}x_2x_3 + 0.25_{(0.1976)}x_1x_2x_3.
\end{aligned}
\tag{2.3}
$$

Table 2.4: Deviations from the target fill height in soft drink bottles

| deviation ($y$) | percent carbonation ($F_1$) | line speed ($F_2$) | operating pressure ($F_3$) |
|---|---|---|---|
| -3 | 10 | 200 | 25 |
| -1 | 10 | 200 | 25 |
| 0 | 12 | 200 | 25 |
| 1 | 12 | 200 | 25 |
| -1 | 10 | 250 | 25 |
| 0 | 10 | 250 | 25 |
| 2 | 12 | 250 | 25 |
| 1 | 12 | 250 | 25 |
| -1 | 10 | 200 | 30 |
| 0 | 10 | 200 | 30 |
| 2 | 12 | 200 | 30 |
| 3 | 12 | 200 | 30 |
| 1 | 10 | 250 | 30 |
| 1 | 10 | 250 | 30 |
| 6 | 12 | 250 | 30 |
| 5 | 12 | 250 | 30 |
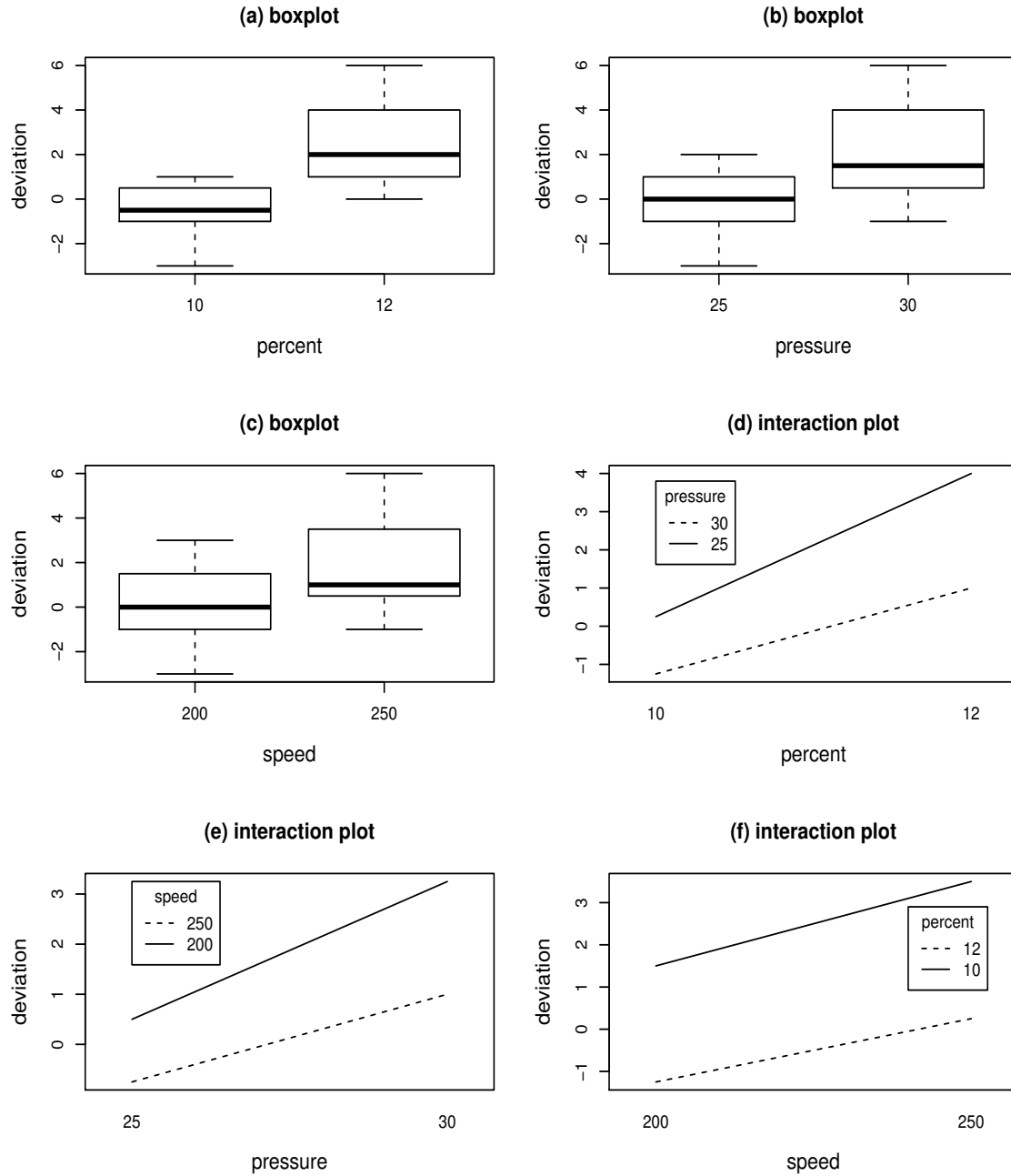
Figure 2.3: Boxplots and interaction plots for Example 2.2: (a) box-plot of deviation versus percent carbonation, (b) box-plot of deviation versus operating pressure, (c) box-plot of deviation versus line speed, (d) an interaction plot between percent and pressure, (e) an interaction plot between pressure and speed, and (f) an interaction plot between speed and percent .

Table 2.5: The effects of three factors with two levels

| run | $F_1$ $(x_1)$ | $F_2$ $(x_2)$ | $F_3$ $(x_3)$ | $F_1F_2$ $(x_1x_2)$ | $F_1F_3$ $(x_1x_3)$ | $F_2F_3$ $(x_2x_3)$ | $F_1F_2F_3$ $(x_1x_2x_3)$ |
|---|---|---|---|---|---|---|---|
| 1 | +1 | +1 | +1 | +1 | +1 | +1 | +1 |
| 2 | −1 | +1 | +1 | −1 | −1 | +1 | −1 |
| 3 | +1 | −1 | +1 | −1 | +1 | −1 | −1 |
| 4 | −1 | −1 | +1 | +1 | −1 | −1 | +1 |
| 5 | +1 | +1 | −1 | +1 | −1 | −1 | −1 |
| 6 | −1 | +1 | −1 | −1 | +1 | −1 | +1 |
| 7 | +1 | −1 | −1 | −1 | −1 | +1 | +1 |
| 8 | −1 | −1 | −1 | +1 | +1 | +1 | −1 |

Since three interactions $x_1x_2$, $x_2x_3$, and $x_1x_2x_3$ are not significant in the full model, a reduced model including the three main effects and the interaction between $F_1$ and $F_3$ is fitted and the result is

$$\hat{y} = 1.00_{(0.203)} + 1.50_{(0.203)}x_1 + 0.875_{(0.203)}x_2 + 1.125_{(0.203)}x_3 + 0.375_{(0.203)}x_1x_3. \quad (2.4)$$

Figure 2.4 shows two plots, the residual versus fitted value, and the normal Q-Q plot. These plots show that it is reasonable to assume equal variance and normal distribution of the errors. From model (2.4), we can conclude that $F_1$, $F_2$, $F_3$ and $F_1F_3$ have significant effects on the fill height. If we perform the partial F test for the full model (2.3) versus reduced model (2.4), the p-value is 0.37 which shows that we can not reject the null hypothesis that all the coefficients for the effects that are not in the reduced model are zero. Thus all the effects that are not in the reduced model are not significant, which implies that the two factor interactions $F_1F_2$ and $F_2F_3$ and the three factor interaction $F_1F_2F_3$ are not significant. Which combination of the

**(a) Residual analysis**
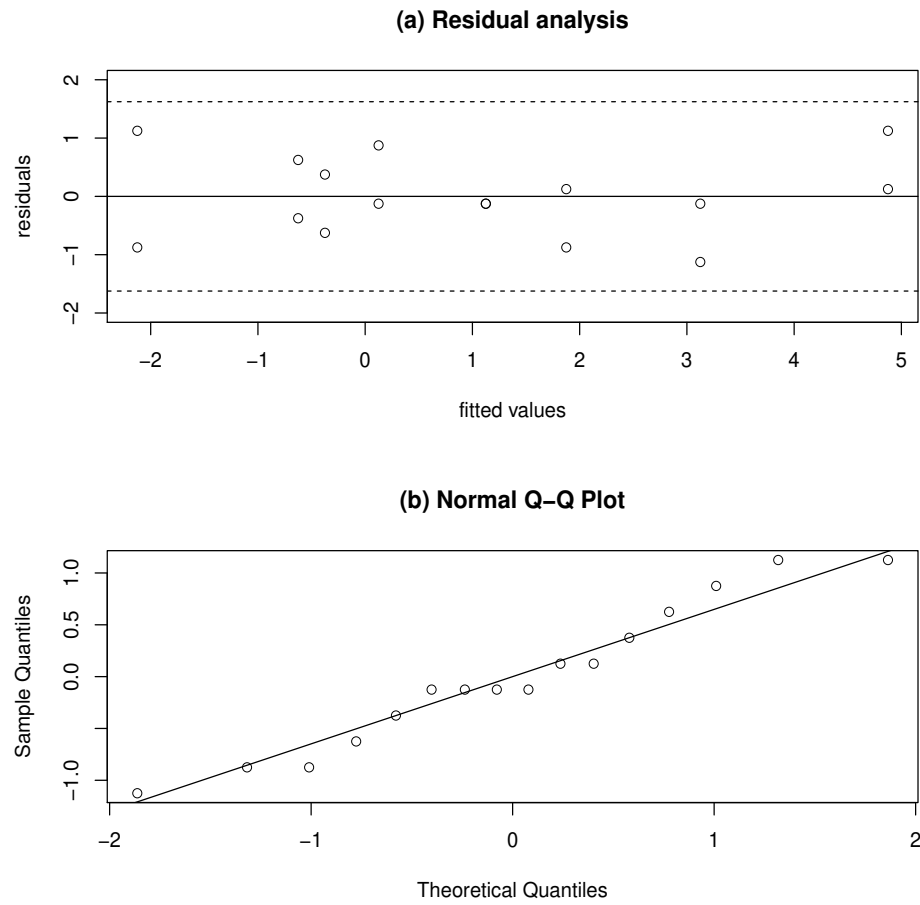
**(b) Normal Q–Q Plot**

Figure 2.4: Residual analysis in the reduced model for Example 2.2: (a) the residual versus fitted value, and (b) the normal Q-Q plot. The dotted horizontal lines are $\pm 2\hat{\sigma}$, where $\hat{\sigma}$ is the estimated standard deviation of the errors.

three factors is the best for both customers and sellers? In other words, we need to find a combination to give zero or nearly zero deviation. Based on the reduced model, there are two choices. One combination is to set 10% for percent carbonation, 250 bpm for line speed and 25 psi for operating pressure, and the other is at 12% for percent carbonation, 200 bpm for line speed and 25 psi for operating pressure.    □

## 2.2   Linear models and requirement set

In Example 2.1, the number of replicates is $r = 4$, and $r = 2$ in Example 2.2. Both examples allow us to fit a full model to analyze all the main effects and interactions. In general, a full model for a factorial design with $r \geq 1$ can be written, in a matrix form, as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\epsilon},$$

where $\mathbf{y}$ is the vector of observed responses, $\mathbf{X}$ is the model matrix, $\boldsymbol{\theta}$ contains the parameters for all the main effects and interactions, and $\boldsymbol{\epsilon}$ is the vector of the random errors which are assumed to have the distribution $N(\mathbf{0}, \sigma^2 \mathbf{I}_n)$ with $n = r\ N$. Here $\mathbf{I}_n$ is the $n \times n$ identity matrix.

For example, the model matrix for $r = 1$ in Example 2.1 is easy to get from Table

2.2,

$$\mathbf{X} = \begin{pmatrix}
1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 \\
1 & -1 & 1 & 0 & -2 & 0 & 0 & 2 & -2 \\
1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 \\
1 & 0 & -2 & -1 & 1 & 0 & 2 & 0 & -2 \\
1 & 0 & -2 & 0 & -2 & 0 & 0 & 0 & 4 \\
1 & 0 & -2 & 1 & 1 & 0 & -2 & 0 & -2 \\
1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 \\
1 & 1 & 1 & 0 & -2 & 0 & 0 & -2 & -2 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{pmatrix},$$

and $\boldsymbol{\theta} = (\theta_0, \theta_1, \cdots, \theta_8)^T$. It is easy to verify that $\mathbf{X}^T\mathbf{X}$ is a diagonal matrix, and

$$\mathbf{X}^T\mathbf{X} = \begin{pmatrix}
9 & & & & & & & & \\
 & 6 & & & & & & & \\
 & & 18 & & & & 0 & & \\
 & & & 6 & & & & & \\
 & & & & 18 & & & & \\
 & & & & & 4 & & & \\
 & & 0 & & & & 12 & & \\
 & & & & & & & 12 & \\
 & & & & & & & & 36
\end{pmatrix}$$

This implies that all the columns of $\mathbf{X}$ are orthogonal.

In Example 2.2, from Table 2.5, the model matrix for $r = 1$ is

$$\mathbf{X} = \begin{pmatrix} 1 & +1 & +1 & +1 & +1 & +1 & +1 & +1 \\ 1 & -1 & +1 & +1 & -1 & -1 & +1 & -1 \\ 1 & +1 & -1 & +1 & -1 & +1 & -1 & -1 \\ 1 & -1 & -1 & +1 & +1 & -1 & -1 & +1 \\ 1 & +1 & +1 & -1 & +1 & -1 & -1 & -1 \\ 1 & -1 & +1 & -1 & -1 & +1 & -1 & +1 \\ 1 & +1 & -1 & -1 & -1 & -1 & +1 & +1 \\ 1 & -1 & -1 & -1 & +1 & +1 & +1 & -1 \end{pmatrix},$$

and $\boldsymbol{\theta} = (\theta_0, \theta_1, \cdots, \theta_7)^T$. It is also easy to verify that $\mathbf{X}^T\mathbf{X}$ is a diagonal matrix, and in fact $\mathbf{X}^T\mathbf{X} = 8\,\mathbf{I}_8$. Therefore all the columns of $\mathbf{X}$ are orthogonal. In general, for a full factorial design, we can always use orthogonal effects in the full model so that $\mathbf{X}^T\mathbf{X}$ is a diagonal matrix.

From Example 2.2, some of the effects are not significant in the full model, so a reduced model can be fitted. We can write the reduced model in a matrix form as

$$\mathbf{y} = \mathbf{X}_1\boldsymbol{\theta}_1 + \boldsymbol{\epsilon}, \tag{2.5}$$

where $\mathbf{y}$ is the vector of observed responses, $\mathbf{X}_1$ is the model matrix, and $\boldsymbol{\theta}_1$ contains the parameters in the reduced model. For model (2.4), $\boldsymbol{\theta}_1 = (\theta_0, \theta_1, \theta_2, \theta_3, \theta_5)^T$, and

$$\mathbf{X}_1 = \begin{pmatrix} 1 & +1 & +1 & +1 & +1 \\ 1 & -1 & +1 & +1 & -1 \\ 1 & +1 & -1 & +1 & +1 \\ 1 & -1 & -1 & +1 & -1 \\ 1 & +1 & +1 & -1 & -1 \\ 1 & -1 & +1 & -1 & +1 \\ 1 & +1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 & +1 \end{pmatrix}.$$

This reduced model is used to study the three main effects and one interaction. A requirement set can be defined to include those effects, say $\mathcal{R} = \{F_1, F_2, F_3, F_1 F_3\}$. In the literature, the requirement set is defined as a subset of effects studied in an experiment (Greenfield, 1976). For a given requirement set, the linear model can be written as a reduced model, such as model (2.5). For a full factorial design, it is clear that the columns of $\mathbf{X}_1$ are also orthogonal.

When there is not enough resource to run a full factorial design in an experiment, a fractional factorial design is often used to screen the factors and identify the influential ones. For a given run size $n$ which is less than $N$, which $n$ combinations do we select to do the experiment? There are $\binom{N}{n}$ choices. Which one is the "optimal" one? We will investigate this in the next chapter.

# Chapter 3
# Optimal design criteria

In this chapter we focus on 2-level fractional factorial designs. For $k$ factors, a full factorial design has $N = 2^k$ runs. When the run size $n$ is less than $N$, how do we choose the $n$ combinations out of the $2^k$ combinations? In Section 3.1, various design criteria to choose optimal designs are reviewed and discussed. In Section 3.2, we introduce a new criterion, A-optimal minimax criterion, which is motivated by the D-optimal minimax criterion in Wilmut and Zhou (2011). Several interesting properties of the A-optimal minimax criterion are derived in Section 3.3.

## 3.1 Optimal design criteria for fractional factorial designs

Various optimal design criteria are proposed and studied in the literature. Many criteria are based on the effect hierarchy principle (Mukerjee and Wu, 2006, p34): "(i) lower order effects are more likely to be important than higher order ones, (ii) factorial effects of the same-order are equally likely to be important." Those criteria include the maximum resolution criterion in Box and Hunter (1961a, b), the minimum aberration criterion in Fries and Hunter (1980), the clear effects criterion in Wu and Chen (1992), and the maximum estimation capacity criterion in Sun (1993). There are other developments in Mukerjee and Wu (2006), Zhang et al. (2008), and Xu, Phoa and Wong (2009). The following examples give some optimal designs using the maximum resolution criterion, the minimum aberration criterion and the clear effects

criterion.

**Example 3.1.** Consider $2^{7-2}$ designs with 7 factors and $n = 32$ runs. The maximum resolution is 4 from Mukerjee and Wu (2006, p54). There are many designs having resolution 4, such as the two designs below

(d1) the $2^{7-2}$ design with the defining relation

$$I = F_1 F_2 F_3 F_4 = F_4 F_5 F_6 F_7 = F_1 F_2 F_3 F_5 F_6 F_7,$$

(d2) the $2^{7-2}$ design with the defining relation

$$I = F_1 F_2 F_3 F_4 = F_3 F_4 F_5 F_6 F_7 = F_1 F_2 F_5 F_6 F_7.$$

The resolution of the above designs can be computed as the length of the shortest word in the defining relation. There are three words in the defining relation in (d1) and (d2). It is obvious that the resolution of (d1) and (d2) is 4, thus both designs (d1) and (d2) are maximum resolution designs. □

**Example 3.2.** Consider the $2^{7-2}$ designs in Example 3.1. The *word length pattern* for a design (d) with $k$ factors is defined as $W(d) = (A_1(d), A_2(d), \cdots, A_k(d))$, where $A_i(d)$ is the number of words with length $i$. For design (d1), it is clear that the word length pattern is $W(d1) = (0, 0, 0, 2, 0, 1, 0)$, while for design (d2), $W(d2) = (0, 0, 0, 1, 2, 0, 0)$. Let $l$ be the smallest integer that $A_l(d1) \neq A_l(d2)$ in the word length patterns. If $A_l(d2) < A_l(d1)$, then (d2) has less aberration than (d1). A design is called a *minimum aberration design* if there exists no other design having less aberration than it. To compare (d1) with (d2), we get $l = 4$ and $A_4(d2) = 1 < A_4(d1) = 2$, thus design (d2) has less aberration than (d1). In fact, design (d2) is a minimum aberration design according to the result in Mukerjee and Wu (2006, p54). □

A fractional factorial design is said to be *regular* if any two effects are either orthogonal or fully aliased; otherwise it is called *non-regular*. A regular fractional

factorial design exists when the run size is a power of 2, such as $n = 4,\ 8,\ 16,\ 32, \cdots$. The designs (d1) and (d2) in Example 3.1 are regular fractional factorial designs with $n = 32$. A fractional factorial design is said to be *orthogonal* if all the main effects are orthogonal. When the run size is a multiple of 4, orthogonal designs can be selected from *Hadamard* matrices. A *Hadamard* matrix is a square matrix and its entries are either $+1$ or $-1$ and its rows are mutually orthogonal. Thus a $n \times n$ matrix $\mathbf{H}$ with all its entries $+1$ and $-1$ is a *Hadamard* matrix if $\mathbf{H}\mathbf{H}^T = \mathbf{H}^T\mathbf{H} = n\mathbf{I}$. The following website contains information about *Hadamard* matrix and lists *Hadamard* matrices for various values of $n$: http://neilsloane.com/hadamard/index.html.

**Example 3.3.** Consider an example from Wu and Chen (1992) for a $2^{6-2}$ design with defining relation as $I = F_1F_2F_5 = F_2F_3F_4F_6 = F_1F_3F_4F_5F_6$. A two-factor interactions (2fi) is *eligible* if it is not aliased with any main effects. Thus $F_1F_2$, $F_1F_5$ and $F_2F_5$ are ineligible since they are aliased with main effects $F_5$, $F_2$ and $F_1$, respectively. And *clear* 2fi's are those eligible ones which are not aliased with other 2fi's. Assuming that interactions involving three and more factors are negligible, the clear 2fi's can be estimated. For this design, the clear 2fi's are $F_1F_3$, $F_1F_4$, $F_1F_6$, $F_3F_5$, $F_4F_5$ and $F_5F_6$.

"A design with less aberration may have a smaller number of eligible 2fi's or of clear 2fi's." (Wu and Chen, 1992). There are various $2^{6-2}$ designs with different resolution, such as the two designs below:

(d3) the $2^{6-2}$ design with the defining relation
$$I = F_1F_2F_3F_5 = F_2F_3F_4F_6 = F_1F_4F_5F_6,$$
(d4) the $2^{6-2}$ design with the defining relation
$$I = F_1F_2F_5 = F_1F_2F_4F_6 = F_4F_5F_6.$$
Design (d3) is the minimum aberration $2^{6-2}$ design with fifteen eligible 2fi's and zero clear 2fi's, and design (d4) has nine eligible 2fi's and five clear 2fi's.  $\square$

Another class of design criteria are model based. Suppose an experimenter wants to fit a pre-specified linear model according to a requirement set, say model (2.5). The least squares estimator (LSE) $\hat{\boldsymbol{\theta}}_1$ of $\boldsymbol{\theta}_1$ is given by

$$\hat{\boldsymbol{\theta}}_1 = \left(\mathbf{X}_1^T \mathbf{X}_1\right)^{-1} \mathbf{X}_1^T \mathbf{y},$$

which has the covariance matrix

$$Cov\left(\hat{\boldsymbol{\theta}}_1\right) = \sigma^2 \left(\mathbf{X}_1^T \mathbf{X}_1\right)^{-1}. \tag{3.1}$$

The A-optimal, D-optimal, and E-optimal designs minimize the trace, determinant and the largest eigenvalue of $Cov\left(\hat{\boldsymbol{\theta}}_1\right)$ respectively. Recently Wilmut and Zhou (2011) proposed a D-optimal minimax criterion to consider both the covariance matrix and the bias of $\hat{\boldsymbol{\theta}}_1$ if the pre-specified linear model is not correct. So the D-optimal minimax criterion is robust against the misspecification of the linear model or the misspecification of the requirement set. Motivated by the D-optimal minimax criterion, we explore an A-optimal minimax criterion and construct A-optimal minimax designs (AOMD) for various cases in this thesis. A-optimal minimax designs will be compared with A-optimal designs (AOD), D-optimal designs (DOD), E-optimal designs (EOD), and D-optimal minimax designs (DOMD).

## 3.2 A-optimal minimax criterion

Suppose the linear model for a given requirement set $\mathcal{R}_0$ with $k$ factors is,

$$\mathbf{y} = \mathbf{X}_1 \boldsymbol{\theta}_1 + \boldsymbol{\epsilon}, \tag{3.2}$$

where $\boldsymbol{\theta}_1$ includes the grand mean and all the parameters for the effects in $\mathcal{R}_0$. Let $p$ be the number of effects in $\mathcal{R}_0$, so $\boldsymbol{\theta}_1 \in R^q$ with $q = p + 1$.

We use $D_{N \times (k+1)}$ to denote design matrix for full factorial design with $k$ factors, and the first column is $\mathbf{1}_N$ for the grand mean term and the $j$th ($j = 2, ..., k + 1$)

column changes its sign every $2^{j-2}$ times. For example, a full factorial design with 3 factors can be expressed as follows:

$$
\mathbf{D} = \begin{pmatrix}
1 & +1 & +1 & +1 \\
1 & -1 & +1 & +1 \\
1 & +1 & -1 & +1 \\
1 & -1 & -1 & +1 \\
1 & +1 & +1 & -1 \\
1 & -1 & +1 & -1 \\
1 & +1 & -1 & -1 \\
1 & -1 & -1 & -1
\end{pmatrix}.
$$

Let $\mathcal{S} = \{\mathbf{u}_1, \cdots, \mathbf{u}_N\}$ be the design space which includes all the $N$ combinations in the full factorial design, where $\mathbf{u}_i$ represents one combination, or one row of full factorial design matrix $D$. We use $\xi_n = \{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n\}$ to denote a design with $n$ design points selected from $\mathcal{S}$ without replacement in this thesis. If the number of points in $\xi_n$ is clear, we can just write $\xi$ for $\xi_n$. Based on $n$ runs, we fit the following model

$$
y_i = \mathbf{z}_{\mathcal{R}_0}^T(\mathbf{x}_i)\boldsymbol{\theta}_1 + \epsilon_i, \quad i = 1, \cdots, n, \tag{3.3}
$$

where $y_i$ is the observed response at the $i$th run, $\mathbf{x}_i$ is a selected combination from the full factorial design, and $\mathbf{z}_{\mathcal{R}_0}^T(\mathbf{x}_i) \in R^q$ is the $i$th row of matrix $\mathbf{X}_1$. For example, for a requirement set $\mathcal{R}_0 = \{F_1, F_2, F_3, F_1F_2\}$ with $k = 3$ and $p = 4$,

$$
\mathbf{z}_{\mathcal{R}_0}(\mathbf{x}_i) = (1, x_{i1}, x_{i2}, x_{i3}, x_{i1}x_{i2})^T,
$$

and $q = 5$.

If the requirement set $\mathcal{R}_0$ missed some significant effects, then model (3.3) is misspecified. We follow the discussion in Wilmut and Zhou (2011) to propose the

possible full model as

$$y_i = \mathbf{z}_{\mathcal{R}_0}^T(\mathbf{x}_i)\boldsymbol{\theta}_1 + h(\mathbf{x}_i) + \epsilon_i, \quad i = 1, \cdots, n, \tag{3.4}$$

where function $h(\mathbf{x}_i)$ is a linear function of all the other effects that are not in $\mathcal{R}_0$, i.e.,

$$h(\mathbf{x}_i) = \mathbf{v}^T(\mathbf{x}_i)\boldsymbol{\theta}_2, \tag{3.5}$$

with $\boldsymbol{\theta}_2 \in R^{N-q}$ being an unknown constant vector and $\mathbf{v}(\mathbf{x}_i)$ being the vector of all the effects not in $\mathcal{R}_0$. For $\mathcal{R}_0 = \{F_1, F_2, F_3, F_1F_2\}$, we have $N - q = 2^3 - 5 = 3$ and

$$\mathbf{v}^T(\mathbf{x}_i) = (x_{i1}x_{i3}, x_{i2}x_{i3}, x_{i1}x_{i2}x_{i3}).$$

From Wilmut and Zhou (2011), $h(\mathbf{x})$ is orthogonal to all the terms in $\mathbf{z}_{\mathcal{R}_0}^T(\mathbf{x})\boldsymbol{\theta}_1$ on the design space $\mathcal{S}$, and $h(\mathbf{x})$ contains all possible departure functions from model (3.3). In order to discuss the bias of the LSE of $\boldsymbol{\theta}_1$, we work on small departure functions, so there is a constraint on $\boldsymbol{\theta}_2$. The constraint is $||\boldsymbol{\theta}_2|| = \sqrt{\boldsymbol{\theta}_2^T\boldsymbol{\theta}_2} \leq \alpha$, where $\alpha \geq 0$ controls the size of departure functions. More detailed discussion is given in Wilmut and Zhou (2011). If $\alpha = 0$, then model (3.3) is correct.

Model (3.4) can be expressed in matrix form as

$$\mathbf{y} = \mathbf{X}_1\boldsymbol{\theta}_1 + \mathbf{X}_2\boldsymbol{\theta}_2 + \boldsymbol{\epsilon}, \tag{3.6}$$

where

$$\mathbf{X}_2 = \begin{pmatrix} \mathbf{v}^T(\mathbf{x}_1) \\ \vdots \\ \mathbf{v}^T(\mathbf{x}_n) \end{pmatrix}.$$

The LSE for $\boldsymbol{\theta}_1$ is given by

$$\hat{\boldsymbol{\theta}}_1 = \left(\mathbf{X}_1^T\mathbf{X}_1\right)^{-1}\mathbf{X}_1^T\mathbf{y},$$

which is estimated from model (3.2). Since the true model is (3.6), the LSE is biased. Its bias and variance are, respectively,

$$
\begin{aligned}
bias(\hat{\boldsymbol{\theta}}_1) &= E(\hat{\boldsymbol{\theta}}_1) - \boldsymbol{\theta}_1 = \left(\mathbf{X}_1^T\mathbf{X}_1\right)^{-1}\mathbf{X}_1^T\mathbf{X}_2\boldsymbol{\theta}_2, \\
Var(\hat{\boldsymbol{\theta}}_1) &= \sigma^2\left(\mathbf{X}_1^T\mathbf{X}_1\right)^{-1}.
\end{aligned}
$$

The mean squared error (MSE) is

$$
\begin{aligned}
MSE(\hat{\boldsymbol{\theta}}_1, \mathbf{X}_1, \boldsymbol{\theta}_2) &= Var(\hat{\boldsymbol{\theta}}_1) + bias(\hat{\boldsymbol{\theta}}_1)bias^T(\hat{\boldsymbol{\theta}}_1) \\
&= \sigma^2\left(\mathbf{X}_1^T\mathbf{X}_1\right)^{-1} + \left(\mathbf{X}_1^T\mathbf{X}_1\right)^{-1}\mathbf{X}_1^T\mathbf{X}_2\boldsymbol{\theta}_2\boldsymbol{\theta}_2^T\mathbf{X}_2^T\mathbf{X}_1\left(\mathbf{X}_1^T\mathbf{X}_1\right)^{-1}.
\end{aligned}
\tag{3.7}
$$

A-optimal, D-optimal and E-optimal designs criteria minimize the variance of the LSE only, so the bias is not considered in these design criteria. In practice, model (3.2) is never true, thus the bias should be considered when constructing optimal designs. Wilmut and Zhou (2011) proposed a D-optimal minimax criterion based on the MSE of the LSE, and a *D-optimal minimax design* minimizes the following loss function

$$
\mathcal{L}_D(\xi_n) = \max_{||\boldsymbol{\theta}_2|| \leq \alpha} \det\left(MSE(\hat{\boldsymbol{\theta}}_1, \mathbf{X}_1, \boldsymbol{\theta}_2)\right),
\tag{3.8}
$$

over possible choices of designs $\xi_n$, which is determined by matrix $\mathbf{X}_1$. This criterion has been extended to fractional factorial designs with mixed levels in Lin and Zhou (2013). D-optimal minimax designs have many nice properties, such as scale invariance and level permutation invariance.

Here we propose an A-optimal minimax criterion and investigate its properties. An *A-optimal minimax design* minimizes the following loss function

$$
\mathcal{L}_A(\xi_n) = \max_{||\boldsymbol{\theta}_2|| \leq \alpha} \text{trace}\left(MSE(\hat{\boldsymbol{\theta}}_1, \mathbf{X}_1, \boldsymbol{\theta}_2)\right),
\tag{3.9}
$$

over possible choices of designs $\xi_n$. Various properties of A-optimal minimax designs are obtained in the next section.

# 3.3 Properties of A-optimal minimax criterion

We deal with minimax problems in both A-optimal and D-optimal minimax criteria. In general, minimax problems are hard to solve analytically and numerically. However, we are able to find analytical solutions for the maximum step in both criteria, which allows us to study many properties of A-optimal and D-optimal minimax designs. First we derive the result for the loss function in (3.9) for the A-optimal minimax criterion, and then we study various properties of A-optimal minimax designs in this section.

**Theorem 1.** *For the loss function in (3.9), we have*

$$\mathcal{L}_A(\xi_n) = \sigma^2 \text{trace}(\mathbf{X}_1^T \mathbf{X}_1)^{-1} + \alpha^2 \left( \frac{N}{\lambda_{\min}(\mathbf{X}_1^T \mathbf{X}_1)} - 1 \right), \tag{3.10}$$

*where $\lambda_{\min}(\cdot)$ denotes the smallest eigenvalue of a matrix.*

**Proof:** Define the following matrices to prove the result. Matrix $\mathbf{W}_1$ is the model matrix for the full factorial design for the requirement set, and matrix $\mathbf{W}_2$ is the model matrix for the complement set of the requirement set, i.e.,

$$\mathbf{W}_1 = \begin{pmatrix} \mathbf{z}_{\mathcal{R}_0}^T(\mathbf{u}_1) \\ \vdots \\ \mathbf{z}_{\mathcal{R}_0}^T(\mathbf{u}_N) \end{pmatrix}, \quad \mathbf{W}_2 = \begin{pmatrix} \mathbf{v}^T(\mathbf{u}_1) \\ \vdots \\ \mathbf{v}^T(\mathbf{u}_N) \end{pmatrix}.$$

Define an $N \times N$ diagonal matrix $\mathbf{M} = diag(n_1, ..., n_N)$, where $n_i = 1$ if the $i$th run is in $\xi_n$, and 0 otherwise. For two-level factorial designs, it is clear that

$$(\mathbf{W}_1, \mathbf{W}_2)^T(\mathbf{W}_1, \mathbf{W}_2) = N\mathbf{I}_N,$$

$$(\mathbf{W}_1, \mathbf{W}_2)(\mathbf{W}_1, \mathbf{W}_2)^T = N\mathbf{I}_N,$$

since all the effects are orthogonal. Also it is easy to verify that

$$\mathbf{X}_1^T\mathbf{X}_1 = \mathbf{W}_1^T\mathbf{M}\mathbf{W}_1,$$

$$\mathbf{X}_1^T\mathbf{X}_2 = \mathbf{W}_1^T\mathbf{M}\mathbf{W}_2.$$

From (3.7) and the above results, we get

$$
\begin{aligned}
\mathcal{L}_A(\xi_n) &= \max_{||\boldsymbol{\theta}_2||\leq\alpha} \ \text{trace}\left(MSE(\hat{\boldsymbol{\theta}}_1, \mathbf{X}_1, \boldsymbol{\theta}_2)\right)\\
&= \max_{||\boldsymbol{\theta}_2||\leq\alpha} \ (\text{trace}(\sigma^2(\mathbf{X}_1^T\mathbf{X}_1)^{-1}) + \text{trace}((\mathbf{X}_1^T\mathbf{X}_1)^{-1}\mathbf{X}_1^T\mathbf{X}_2\boldsymbol{\theta}_2\boldsymbol{\theta}_2^T\mathbf{X}_2^T\mathbf{X}_1(\mathbf{X}_1^T\mathbf{X}_1)^{-1}))\\
&= \max_{||\boldsymbol{\theta}_2||\leq\alpha} \ (\sigma^2\text{trace}(\mathbf{X}_1^T\mathbf{X}_1)^{-1} + \text{trace}(\boldsymbol{\theta}_2^T\mathbf{X}_2^T\mathbf{X}_1(\mathbf{X}_1^T\mathbf{X}_1)^{-2}\mathbf{X}_1^T\mathbf{X}_2\boldsymbol{\theta}_2))\\
&= \max_{||\boldsymbol{\theta}_2||\leq\alpha} \ (\sigma^2\text{trace}(\mathbf{X}_1^T\mathbf{X}_1)^{-1} + \boldsymbol{\theta}_2^T\mathbf{X}_2^T\mathbf{X}_1(\mathbf{X}_1^T\mathbf{X}_1)^{-2}\mathbf{X}_1^T\mathbf{X}_2\boldsymbol{\theta}_2)\\
&= \sigma^2\text{trace}(\mathbf{X}_1^T\mathbf{X}_1)^{-1} + \alpha^2\lambda_{\max}(\mathbf{X}_2^T\mathbf{X}_1(\mathbf{X}_1^T\mathbf{X}_1)^{-2}\mathbf{X}_1^T\mathbf{X}_2)\\
&= \sigma^2\text{trace}(\mathbf{X}_1^T\mathbf{X}_1)^{-1} + \alpha^2\lambda_{\max}((\mathbf{X}_1^T\mathbf{X}_1)^{-2}\mathbf{X}_1^T\mathbf{X}_2\mathbf{X}_2^T\mathbf{X}_1)\\
&= \sigma^2\text{trace}(\mathbf{X}_1^T\mathbf{X}_1)^{-1} + \alpha^2\lambda_{\max}((\mathbf{W}_1^T\mathbf{M}\mathbf{W}_1)^{-2}\mathbf{W}_1^T\mathbf{M}\mathbf{W}_2\mathbf{W}_2^T\mathbf{M}\mathbf{W}_1)\\
&= \sigma^2\text{trace}(\mathbf{X}_1^T\mathbf{X}_1)^{-1} + \alpha^2\lambda_{\max}((\mathbf{W}_1^T\mathbf{M}\mathbf{W}_1)^{-2}\mathbf{W}_1^T\mathbf{M}(N\mathbf{I} - \mathbf{W}_1\mathbf{W}_1^T)\mathbf{M}\mathbf{W}_1)\\
&= \sigma^2\text{trace}(\mathbf{X}_1^T\mathbf{X}_1)^{-1} + \alpha^2\lambda_{\max}((\mathbf{W}_1^T\mathbf{M}\mathbf{W}_1)^{-2}(N\mathbf{W}_1^T\mathbf{M}\mathbf{W}_1 - \mathbf{W}_1^T\mathbf{M}\mathbf{W}_1\mathbf{W}_1^T\mathbf{M}\mathbf{W}_1))\\
&= \sigma^2\text{trace}(\mathbf{X}_1^T\mathbf{X}_1)^{-1} + \alpha^2\lambda_{\max}(N(\mathbf{W}_1^T\mathbf{M}\mathbf{W}_1)^{-1} - \mathbf{I})\\
&= \sigma^2\text{trace}(\mathbf{X}_1^T\mathbf{X}_1)^{-1} + \alpha^2\left(\frac{N}{\lambda_{\min}(\mathbf{X}_1^T\mathbf{X}_1)} - 1\right),
\end{aligned}
$$

where $\lambda_{\max}(\cdot)$ denotes the largest eigenvalue of a matrix. This completes the proof.

□

A similar result is derived for the D-optimal minimax criterion in Wilmut and Zhou (2011), and the result is

$$\mathcal{L}_D(\xi_n) = \sigma^{2q}\frac{1 + \frac{\alpha^2}{\sigma^2}(N - \lambda_{\min}(\mathbf{X}_1^T\mathbf{X}_1))}{\det(\mathbf{X}_1^T\mathbf{X}_1)}. \tag{3.11}$$

From these results in (3.10) and (3.11), various properties of A-optimal minimax designs can be studied, and A-optimal minimax designs can be compared with A-optimal, D-optimal and E-optimal designs and D-optimal minimax designs. Define

$$A(\xi_n) = \text{trace}\left(\mathbf{X}_1^T\mathbf{X}_1\right)^{-1}, \tag{3.12}$$

$$D(\xi_n) = \det\left(\mathbf{X}_1^T\mathbf{X}_1\right)^{-1}, \tag{3.13}$$

$$E(\xi_n) = \lambda_{\max}\left(\left(\mathbf{X}_1^T\mathbf{X}_1\right)^{-1}\right). \tag{3.14}$$

A-optimal, D-optimal and E-optimal designs minimize $A(\xi_n), D(\xi_n)$ and $E(\xi_n)$ respectively. Suppose $\lambda_1 \geq \cdots \geq \lambda_q$ are the $q$ ordered eigenvalues of $\mathbf{X}_1^T\mathbf{X}_1$, then the $q$ eigenvalues of $\left(\mathbf{X}_1^T\mathbf{X}_1\right)^{-1}$ are: $1/\lambda_1, \cdots, 1/\lambda_q$. From (3.10) – (3.14), we have

$$\mathcal{L}_A(\xi_n) = \sigma^2\left(\frac{1}{\lambda_1} + \cdots + \frac{1}{\lambda_q}\right) + \alpha^2\left(\frac{N}{\lambda_q} - 1\right),$$

$$\mathcal{L}_D(\xi_n) = \sigma^{2q}\frac{1 + \frac{\alpha^2}{\sigma^2}(N - \lambda_q)}{\lambda_1 \cdots \lambda_q},$$

$$A(\xi_n) = \frac{1}{\lambda_1} + \cdots + \frac{1}{\lambda_q},$$

$$D(\xi_n) = \frac{1}{\lambda_1 \cdots \lambda_q},$$

$$E(\xi_n) = \frac{1}{\lambda_q}.$$

It is clear that all the loss functions are functions of the eigenvalues of $\mathbf{X}_1^T\mathbf{X}_1$.

**Lemma 1.** *All the eigenvalues of $\mathbf{X}_1^T\mathbf{X}_1$ stay the same if the two levels of one factor or several factors are switched in $\mathbf{X}_1$.*

**Proof:** If we switch the two levels of one factor, say $F_1$, that is changing $+1$ to $-1$ and $-1$ to $+1$ in the corresponding columns in $\mathbf{X}_1$, and all the other factors stay the same. The new design matrix is denoted as $\hat{\mathbf{X}}_1$, in which the sign for $F_1$ and all the interactions related to $F_1$ are changed. It is clear that

$$\hat{\mathbf{X}}_1 = \mathbf{X}_1\mathbf{Q}_1$$

where $\mathbf{Q}_1 = diag\{1, q_1, q_2, \cdots, q_p\}$ is a diagonal matrix, and $q_{i-1} = -1$ if the $i$th column is changed, and $q_{i-1} = 1$ otherwise. It is obvious that

$$\mathbf{Q}_1^T = \mathbf{Q}_1, \quad \mathbf{Q}_1^2 = \mathbf{I}_q.$$

Therefore $\hat{\mathbf{X}}_1^T \hat{\mathbf{X}}_1 = \mathbf{Q}_1 \mathbf{X}_1^T \mathbf{X}_1 \mathbf{Q}_1$ and all the eigenvalues of $\mathbf{Q}_1 \mathbf{X}_1^T \mathbf{X}_1 \mathbf{Q}_1$ are the same as those of $\mathbf{X}_1^T \mathbf{X}_1$. Similarly if we change the sign of several factors, we just need to change the sign of corresponding columns of $\mathbf{Q}_1$ and still get the same result. □

This property implies that all the optimal designs are invariant under level permutation, so the classification of the two levels is not important. In practice this situation happens. For example, it doesn't matter how to define high and low levels for two different material types.

**Lemma 2.** *All the loss functions, $A(\xi_n), D(\xi_n), E(\xi_n), \mathcal{L}_A(\xi_n)$ and $\mathcal{L}_D(\xi_n)$ are minimized when $\mathbf{X}_1^T \mathbf{X}_1 = n\mathbf{I}_q$.*

**Proof:** We only prove the result for $\mathcal{L}_A(\xi_n)$ here. The other results are known or can be proved similarly. From Theorem 1, we have

$$\mathcal{L}_A(\xi_n) = \sigma^2 \left( \frac{1}{\lambda_1} + \cdots + \frac{1}{\lambda_q} \right) + \alpha^2 \left( \frac{N}{\lambda_q} - 1 \right).$$

For any $\mathbf{X}_1$, we have trace $\left( \mathbf{X}_1^T \mathbf{X}_1 \right) = nq = \sum_{i=1}^q \lambda_i$. Since the geometric mean of a set of numbers is less than the set's arithmetic mean unless all the members are equal, we have

$$\sqrt[q]{\prod_{i=1}^q \lambda_i} \leq \frac{1}{q} \sum_{i=1}^q \lambda_i = n, \tag{3.15}$$

and

$$\sqrt[q]{\prod_{i=1}^q \frac{1}{\lambda_i}} \leq \frac{1}{q} \sum_{i=1}^q \frac{1}{\lambda_i}. \tag{3.16}$$

From (3.15), we get

$$\frac{1}{\sqrt[q]{\prod_{i=1}^{q} \lambda_i}} \geq \frac{1}{n} \; . \tag{3.17}$$

Combining (3.16) with (3.17) gives

$$\frac{1}{n} \leq \sqrt[q]{\prod_{i=1}^{q} \frac{1}{\lambda_i}} \leq \frac{1}{q} \sum_{i=1}^{q} \frac{1}{\lambda_i} \; . \tag{3.18}$$

The equality holds only in the case of all $\frac{1}{\lambda_i}$ are equal.

Also, since $\lambda_q$ is the smallest eigenvalue of $\mathbf{X}_1^T \mathbf{X}_1$, from $\sum_{i=1}^{q} \lambda_i = nq$ we have

$$\lambda_q \leq n, \quad \frac{1}{\lambda_q} \geq \frac{1}{n}.$$

Therefore

$$\mathcal{L}_A(\xi_n) = \sigma^2 \sum_{i=1}^{q} \frac{1}{\lambda_i} + \frac{N\alpha^2}{\lambda_q} - \alpha^2 \geq \frac{\sigma^2 q}{n} + \frac{N\alpha^2}{n} - \alpha^2. \tag{3.19}$$

When $\mathbf{X}_1^T \mathbf{X}_1 = n\mathbf{I}_q$, $\lambda_i = n$ and $\frac{1}{\lambda_i} = \frac{1}{n}$, for all $i = 1, \cdots, q$. Thus $\sum_{i=1}^{q} \frac{1}{\lambda_i}$ and $\frac{1}{\lambda_q}$ reach their lower bounds at the same time, and $\mathcal{L}_A(\xi_n) = \sigma^2 \frac{q}{n} + \alpha^2(\frac{N}{n} - 1)$, which gives the lower bound of the loss function for AOMD. $\qquad \square$

Lemma 2 implies that if a design with design matrix $\mathbf{X}_1$ satisfying $\mathbf{X}_1^T \mathbf{X}_1 = n\mathbf{I}_q$, the design is AOD, DOD, EOD, AOMD and DOMD. For a requirement set $\mathcal{R}$, if $\mathbf{X}_1^T \mathbf{X}_1 = n\mathbf{I}_q$, then the design is called an orthogonal design for $\mathcal{R}$. For some $n$ and requirement sets, there may exist orthogonal designs for $\mathcal{R}$. However, in many situations, such a $\mathbf{X}_1$ does not exist, and the following Lemma 3 and Theorem 2 provide a couple of cases.

**Lemma 3.** *For any design with* $n = N - 1$, $\mathbf{X}_1^T \mathbf{X}_1$ *has eigenvalues* $\lambda_1 = N, \cdots,$ $\lambda_{q-1} = N, \lambda_q = N - q.$

**Proof:** For $n = N - 1$, assuming the $\mathbf{u}_j$ is omitted from the design, we have

$$\mathbf{X}_1^T \mathbf{X}_1 = \sum_{i=1}^{N} \mathbf{z}(\mathbf{u}_i) \mathbf{z}^T(\mathbf{u}_i) - \mathbf{z}(\mathbf{u}_j) \mathbf{z}^T(\mathbf{u}_j) = N\mathbf{I}_q - \mathbf{z}(\mathbf{u}_j) \mathbf{z}^T(\mathbf{u}_j).$$

For the matrix like this type, the $q$ eigenvalues are $N, \cdots, N$, and $N - \mathbf{z}^T(\mathbf{u}_j) \mathbf{z}(\mathbf{u}_j) = N - q$. $\quad\square$

As we discussed before, all the loss functions are based on the eigenvalues of $\mathbf{X}_1^T \mathbf{X}_1$. From Lemma 3, if we just remove one combination from the full factorial design, all the designs are equivalent since the eigenvalues of $\mathbf{X}_1^T \mathbf{X}_1$ for all the designs are the same. In this case, It is obvious that $\mathbf{X}_1^T \mathbf{X}_1 \neq n\mathbf{I}_q$. Furthermore, we have the following result.

**Theorem 2.** *For $N - q < n \leq N - 1$, there doesn't exist any design with $\mathbf{X}_1^T \mathbf{X}_1 = n\mathbf{I}_q$.*

**Proof:** From Lemma 3 we know that, for $n = N - 1$,

$$\lambda_{\min}(\mathbf{X}_1^T \mathbf{X}_1) = N - q.$$

Since the smallest eigenvalue decreases as $n$ decreases (Wilmut and Zhou, 2011), for $N - q < n \leq N - 1$,

$$\lambda_{\min}(\mathbf{X}_1^T \mathbf{X}_1) \leq N - q. \tag{3.20}$$

If there exists a design satisfying $\mathbf{X}_1^T \mathbf{X}_1 = nI_q$, which means all the eigenvalues are equal to $n$, then $\lambda_{\min}(\mathbf{X}_1^T \mathbf{X}_1) = n > N - q$, which is a contradiction to (3.20). Therefore, for $N - q < n \leq N - 1$, there doesn't exist any design with $\mathbf{X}_1^T \mathbf{X}_1 = n\mathbf{I}_q$. $\quad\square$

**Theorem 3.** *For $q \leq n \leq N$, we have,*

$$\sigma^2 \frac{q}{n} + \alpha^2 \left(\frac{N}{n} - 1\right) \leq \min_{\xi_n} \mathcal{L}_A(\xi_n) \leq \min_{\xi_{n-1}} \mathcal{L}_A(\xi_{n-1}).$$

**Proof:** Similar to the proof of Lemma 2 in Wilmut and Zhou (2011), we can define an add-one new design $\xi_{n,1}$ including all the combinations in design $\xi_{n-1}^*$ and one more combination, where design $\xi_{n-1}^*$ minimizes the $\mathcal{L}_A(\xi_{n-1})$. The minimum eigenvalue of the matrix for design $\xi_{n-1}^*$ is not larger than the one for design $\xi_{n,1}$. And the trace of $(\mathbf{X}_1^T \mathbf{X}_1)^{-1}$ for design $\xi_{n-1}^*$ is not smaller than the one for design $\xi_{n,1}$. Thus we have $\mathcal{L}_A(\xi_{n,1}) \leq \mathcal{L}_A(\xi_{n-1}^*)$, which leads to

$$\min_{\xi_n} \mathcal{L}_A(\xi_n) \leq \mathcal{L}_A(\xi_{n,1}) \leq \mathcal{L}_A(\xi_{n-1}^*) = \min_{\xi_{n-1}} \mathcal{L}_A(\xi_{n-1}).$$

The lower bound for $\min_{\xi_n} \mathcal{L}_A(\xi_n)$ can be seen from (3.19) in the proof of Lemma 2.

$\square$

There are various criteria to choose the "optimal" designs. We are curious to study if there is any difference among all the criteria. Are AOD, DOD, EOD, AOMD and DOMD the same? Several examples will be given to find optimal designs for various criteria in the next chapter, and these optimal designs are compared.

# Chapter 4

# Optimal fractional factorial designs

In this chapter, we construct optimal designs for various criteria and various requirement sets and compare those optimal designs. Section 4.1 provides a list of numbers for the $N$ runs of a full factorial design with $k$ factors, and the numbers will be used to present optimal designs. Section 4.2 gives two search algorithms to compute optimal designs, a complete search algorithm and an annealing algorithm. Section 4.3 contains various optimal designs from the complete search algorithm and guidelines to find optimal designs. Section 4.4 presents some optimal designs from the annealing algorithm and compares those optimal designs.

## 4.1  A standard list of a full factorial design

There are $N = 2^k$ runs in a full factorial design with $k$ factors, $F_1, F_2, \cdots, F_k$. We use numbers $1, 2, \cdots, N$ to represent the $N$ runs. The numbers are generated as follows and will be used to present optimal fractional factorial designs. Starting at the first run, all the factors are at the low level, and factor $F_j$ alternates between the low $(-)$ and high $(+)$ levels for every $2^{j-1}$ runs, $j = 1, \cdots, k$. For example, Table 4.1 gives the numbers and factor levels for 4 factors with 16 runs.

## 4.2  Numerical algorithms

For some requirement sets and run size $n$, optimal designs can be constructed using the properties discussed in Chapter 3. However, optimal designs often need

Table 4.1: The 16 runs of the $2^4$ full factorial design.

| Run | $F_1$ | $F_2$ | $F_3$ | $F_4$ |
|---|---|---|---|---|
| 1 | − | − | − | − |
| 2 | + | − | − | − |
| 3 | − | + | − | − |
| 4 | + | + | − | − |
| 5 | − | − | + | − |
| 6 | + | − | + | − |
| 7 | − | + | + | − |
| 8 | + | + | + | − |
| 9 | − | − | − | + |
| 10 | + | − | − | + |
| 11 | − | + | − | + |
| 12 | + | + | − | + |
| 13 | − | − | + | + |
| 14 | + | − | + | + |
| 15 | − | + | + | + |
| 16 | + | + | + | + |

to be computed numerically. There are $\binom{N}{n}$ possible fractional factorial designs. If $N$ and $n$ are small, a complete search algorithm is feasible which finds optimal designs by computing the loss function for all possible fractional factorial designs. An optimal design has the smallest value of a loss function. For moderate and large $N$ and $n$, $\binom{N}{n}$ can be huge, and a complete search algorithm may not be feasible. An annealing algorithm is shown to be effective to search for optimal and robust designs, for example, see Fang & Wiens (2000), Zhou (2001, 2008), and Wilmut & Zhou (2011). More details about a simulated annealing algorithm can be found in Givens & Hoeting (2005). There are many other algorithms to compute optimal designs, for example, see Lu & Pong (2013) and Yu (2010, 2011).

Annealing algorithm is a random search technique for optimal solution, which is an analogy of natural phenomenon. We simulate the annealing process of a metal cooling and freezing into a crystalline structure and apply it into searching for optimal result in general problems. The description of an annealing algorithm for computing optimal fractional factorial designs is given by Wilmut & Zhou (2011). The algorithm is denoted as $\text{ALA}(m_0, T_0, iterT_0, iter)$, where $m_0$ is the maximum number of runs that are allowed to be changed in one search, $T_0$ is the initial temperature, $iterT_0$ is the total number of changes in temperature, and $iter$ is the total number of designs searched at each temperature. The main idea is to get an initial design $\xi_n^{(0)}$, make a small change to $\xi_n^{(0)}$ and get a new design $\xi_n^{(1)}$ if it is accepted, and continue this process to produce a sequence of designs, $\xi_n^{(1)}, \xi_n^{(2)}, \xi_n^{(3)}, \cdots$. The limiting design is considered as an optimal design. The parameters $m_0, T_0, iterT_0, iter$ in the algorithm control the small change, the acceptance criterion and stopping criterion, and they need to be adjusted for each optimization problem.

Suppose we minimize a loss function $\mathcal{L}(\xi)$ to find an optimal design of $n$ runs. The detailed steps of the annealing algorithm are given as follows:

(1) Randomly choose an initial design $\xi^{(0)}$ and calculate the loss function for this design $\mathcal{L}(\xi^{(0)})$. Set an iteration number $jj = 1$.

(2) For each $T_0$, select a number from $\{1, 2, ..., m_0\}$ randomly, denoted by $a_0$. A new design $\xi^{new}$ is obtained by selecting $a_0$ runs from the $N - n$ runs which are not in design $\xi^{(0)}$ to replace $a_0$ randomly selected runs in $\xi^{(0)}$.

(3) Compute the loss function for $\xi^{new}$. If $\mathcal{L}(\xi^{new}) \leq \mathcal{L}(\xi^{(0)})$, then let $\xi^{(0)} = \xi^{new}$. If $\mathcal{L}(\xi^{new}) \geq \mathcal{L}(\xi^{(0)})$, $\xi^{(0)} = \xi^{new}$ with probability $pp = exp(-(\mathcal{L}(\xi^{new}) - \mathcal{L}(\xi^{(0)}))/T_0)$. Otherwise $\xi^{(0)}$ stays the same. Repeat steps (2) and (3) for $iter$ times.

(4) Reduce the temperature using $T_0 = 0.9T_0$ and set $jj = jj + 1$. If $jj \leq iterT_0$, go to step (2). Otherwise go to step (5).

(5) The design $\xi^{(0)}$ at the end is viewed as the limiting design and considered to be an optimal design.

We need to select parameters $m_0$, $T_0$, $iterT_0$ and $iter$ carefully. A large $T_0$ gives high probabilities to accept a new design at the beginning and it may take many iterations for the designs to converge. A small $T_0$ may yield a local optimal solution. A large $iterT_0$ is needed to make sure that the loss function converges. Parameter $iter$ should be large enough to make sure that we do many searches at each temperature. The total number of designs searched is $iterT_0 \times iter$. We set $m_0 = 5$ in the examples in this chapter and it works well. In practice, we often run the algorithm several times to see if it yields limiting designs with the same loss function value. Notice that optimal designs are usually not unique, so the limiting designs may not be the same but their loss function value should be the same.

## 4.3 Optimal designs from the complete search algorithm

All the results in this section are obtained from the complete search algorithm. We define a ratio parameter as $\nu = \frac{\alpha^2}{\sigma^2}$. We assume $\nu = 1$ for loss functions of AOMD and DOMD. Actually, the choice of the ratio parameter doesn't matter if AOMD (DOMD) are also AOD (DOD) and EOD. In the following examples, we use $\xi_A$, $\xi_{LA}$, $\xi_E$, $\xi_D$ and $\xi_{LD}$ to denote AOD, AOMD, EOD, DOD and DOMD.

**Example 4.1**. Consider the requirement set $\mathcal{R} = \{F_1, F_2, F_3, F_4, F_1 F_2\}$ with $k = 4$. The AOMD and DOMD designs are computed for run size $n = 8, 9, ..., 16$. There are many optimal designs for each $n$, and AOMD and DOMD are equivalent. One optimal design for each run size is presented in Table 4.2, and the results show that the loss functions for AOMD and DOMD are decreasing as $n$ increases, which is consistent with the result in Theorem 3 and from Wilmut and Zhou (2011).

There are two plots in Figure 4.1. (a) $min_{\xi_n} \mathcal{L}_A(\xi_n)$ versus $n$, (b) $min_{\xi_n} \mathcal{L}_D(\xi_n)^{1/q}$ versus $n$. We can see that the loss functions for both AOMD and DOMD are decreasing as run size $n$ increases. For $n = 8$, the optimal design is orthogonal for $\mathcal{R}$, while for $9 \leq n \leq 15$, the optimal designs are not orthogonal. $\square$

**Example 4.2**. Consider the requirement set $\mathcal{R} = \{F_1, F_2, F_3, F_4\}$ with $k = 4$. The AOD, AOMD, EOD, DOD and DOMD designs are computed for run size $n = 8$ and $n = 12$. We get the following results from the computation: (a) All the AOD, AOMD, EOD, DOD and DOMD are the same; (b) There are 10 optimal designs for run size $n = 8$ and 120 for $n = 12$; (c) Table 4.3 gives one optimal design for $n = 8$ and one for $n = 12$. For $n = 8$, the design is orthogonal, i.e, $\mathbf{X}_1^T \mathbf{X}_1 = n \mathbf{I}_q$. (d) For $n = 12$, there doesn't exist a design with $\mathbf{X}_1^T \mathbf{X}_1 = n \mathbf{I}_q$, since $n = 12 > N - q = 11$. This is consistant with the result in Theorem 2.

Table 4.2: AOMD and DOMD in Example 4.1: The numbers in optimal designs are the row numbers from Table 4.1.

| run size $n$ | optimal designs | $\mathcal{L}_A(\xi_n)$ | $\mathcal{L}_D(\xi_n)^{1/q}$ |
|:---:|:---|:---:|:---:|
| 8 | 1,2,7,8,11,12,13,14 | 1.7500 | 0.1803 |
| 9 | 1,2,3,5,8,9,12,14,15 | 1.6964 | 0.1642 |
| 10 | 1,2,3,5,6,8,9,12,14,15 | 1.6429 | 0.1496 |
| 11 | 1,2,3,4,5,6,7,9,10,15,16 | 1.5923 | 0.1367 |
| 12 | 1,2,3,4,5,6,7,8,9,10,15,16 | 1.5417 | 0.1250 |
| 13 | 1,2,3,4,5,6,7,8,9,10,11,13,16 | 1.4958 | 0.1148 |
| 14 | 1,2,3,4,5,6,7,8,9,10,11,13,14,16 | 1.0500 | 0.1011 |
| 15 | 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15 | 1.0125 | 0.0935 |
| 16 | 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16 | 0.3750 | 0.0625 |

Table 4.3: AOD, AOMD, EOD, DOD and DOMD for $\mathcal{R} = \{F_1, F_2, F_3, F_4\}$

| run size $n$ | optimal designs | $A(\xi_n)$ | $\mathcal{L}_A(\xi_n)$ | $E(\xi_n)$ | $D(\xi_n)^{1/q}$ | $\mathcal{L}_D(\xi_n)^{1/q}$ |
|:---:|:---|:---:|:---:|:---:|:---:|:---:|
| 8 | 1,2,7,8,11,12,13,14 (orthogonal design) | 0.6250 | 1.7500 | 0.1250 | 0.1250 | 0.1940 |
| 12 | 1,2,3,4,5,6,7,8,9,12,14,15 (not orthogonal design) | 0.4375 | 1.4375 | 0.1250 | 0.0853 | 0.1324 |

**(a) AOMD**



**(b) DOMD**
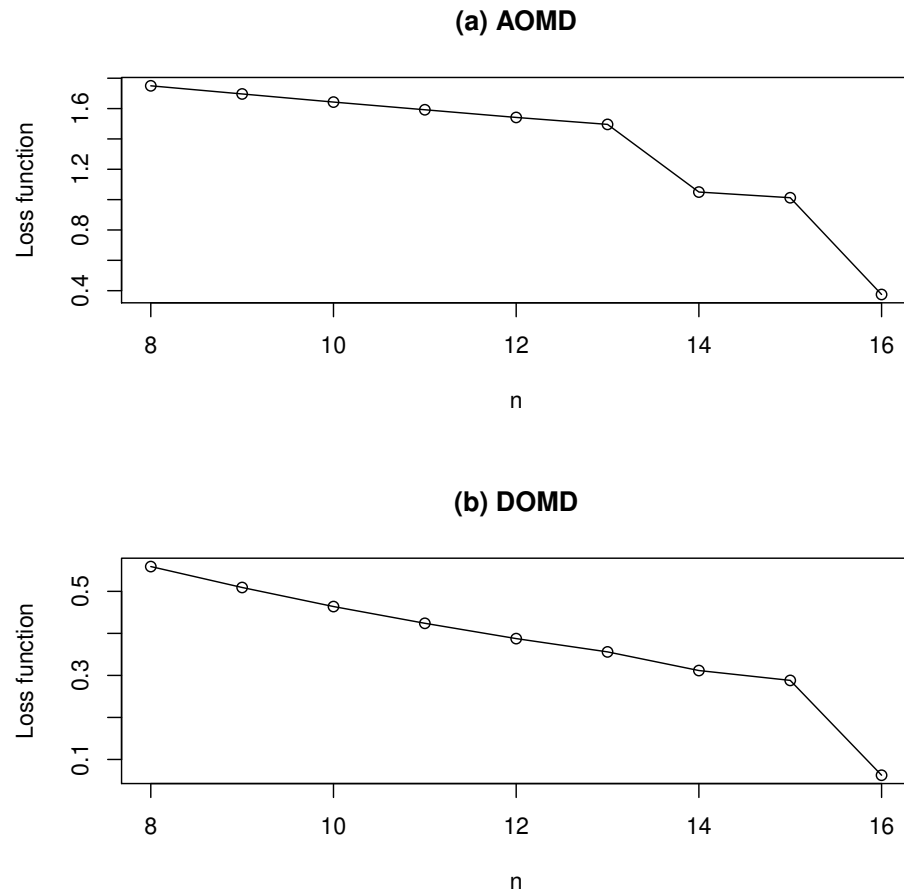


Figure 4.1: Plots of loss functions: (a) $min_{\xi_n}\mathcal{L}_A(\xi_n)$ versus $n$, (b) $min_{\xi_n}\mathcal{L}_D(\xi_n)^{1/q}$ versus $n$.

For $n = 8$, the design matrix $\mathbf{X}_1$ and $\mathbf{X}_1^T\mathbf{X}_1$ are, respectively,

$$\mathbf{X}_1 = \begin{pmatrix} 1 & -1 & -1 & -1 & -1 \\ 1 & +1 & -1 & -1 & -1 \\ 1 & -1 & +1 & +1 & -1 \\ 1 & +1 & +1 & +1 & -1 \\ 1 & -1 & +1 & -1 & +1 \\ 1 & +1 & +1 & -1 & +1 \\ 1 & -1 & -1 & +1 & +1 \\ 1 & +1 & -1 & +1 & +1 \end{pmatrix},$$

$$\mathbf{X}_1^T\mathbf{X}_1 = \begin{pmatrix} 8 & 0 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 & 0 \\ 0 & 0 & 8 & 0 & 0 \\ 0 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 0 & 8 \end{pmatrix} = 8\mathbf{I}_5,$$

For $n = 12$, the design matrix $\mathbf{X}_1$ and $\mathbf{X}_1^T\mathbf{X}_1$ are, respectively,

$$\mathbf{X}_1 = \begin{pmatrix} 1 & -1 & -1 & -1 & -1 \\ 1 & +1 & -1 & -1 & -1 \\ 1 & -1 & +1 & -1 & -1 \\ 1 & +1 & +1 & -1 & -1 \\ 1 & -1 & -1 & +1 & -1 \\ 1 & +1 & -1 & +1 & -1 \\ 1 & -1 & +1 & +1 & -1 \\ 1 & +1 & +1 & +1 & -1 \\ 1 & -1 & -1 & -1 & +1 \\ 1 & +1 & +1 & -1 & +1 \\ 1 & +1 & -1 & +1 & +1 \\ 1 & -1 & +1 & +1 & +1 \end{pmatrix},$$

$$\mathbf{X}_1^T\mathbf{X}_1 = \begin{pmatrix} 12 & 0 & 0 & 0 & -4 \\ 0 & 12 & 0 & 0 & 0 \\ 0 & 0 & 12 & 0 & 0 \\ 0 & 0 & 0 & 12 & 0 \\ -4 & 0 & 0 & 0 & 12 \end{pmatrix} \neq 12\mathbf{I}_5,$$

If we change the requirement set to $\mathcal{R} = \{F_1, F_2, F_3, F_4, F_1F_2, F_2F_3\}$, the results are shown in Table 4.4.

Table 4.4: AOD, AOMD, EOD, DOD and DOMD for $\mathcal{R} = \{F_1, F_2, F_3, F_4, F_1F_2, F_2F_3\}$

| run size $n$ | optimal designs | $A(\xi_n)$ | $\mathcal{L}_A(\xi_n)$ | $E(\xi_n)$ | $D(\xi_n)^{1/q}$ | $\mathcal{L}_D(\xi_n)^{1/q}$ |
|---|---|---|---|---|---|---|
| 8 | 1,3,6,8,10,12,13,15 (orthogonal design) | 0.8750 | 1.8750 | 0.1250 | 0.1250 | 0.1711 |
| 12 | 1,2,3,4,5,6,7,8,9,11,14,16 (non-orthogonal design) | 0.6458 | 1.6458 | 0.1250 | 0.0876 | 0.1200 |

For $n = 8$, the design matrix $\mathbf{X}_1$ and $\mathbf{X}_1^T\mathbf{X}_1$ are, respectively,

$$\mathbf{X}_1 = \begin{pmatrix} 1 & -1 & -1 & -1 & -1 & +1 & +1 \\ 1 & -1 & +1 & -1 & -1 & -1 & -1 \\ 1 & +1 & -1 & +1 & -1 & -1 & -1 \\ 1 & +1 & +1 & +1 & -1 & +1 & +1 \\ 1 & +1 & -1 & -1 & +1 & -1 & +1 \\ 1 & +1 & +1 & -1 & +1 & +1 & -1 \\ 1 & -1 & -1 & +1 & +1 & +1 & -1 \\ 1 & -1 & +1 & +1 & +1 & -1 & +1 \end{pmatrix},$$

$$\mathbf{X}_1^T\mathbf{X}_1 = \begin{pmatrix} 8 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 8 \end{pmatrix} = 8\mathbf{I}_7,$$

For $n = 12$, the design matrix $\mathbf{X}_1$ and $\mathbf{X}_1^T\mathbf{X}_1$ are, respectively,

$$\mathbf{X}_1 = \begin{pmatrix}
1 & -1 & -1 & -1 & -1 & +1 & +1 \\
1 & +1 & -1 & -1 & -1 & -1 & +1 \\
1 & -1 & +1 & -1 & -1 & -1 & -1 \\
1 & +1 & +1 & -1 & -1 & +1 & -1 \\
1 & -1 & -1 & +1 & -1 & +1 & -1 \\
1 & +1 & -1 & +1 & -1 & -1 & -1 \\
1 & -1 & +1 & +1 & -1 & -1 & +1 \\
1 & +1 & +1 & +1 & -1 & +1 & +1 \\
1 & -1 & -1 & -1 & +1 & +1 & +1 \\
1 & -1 & +1 & -1 & +1 & -1 & -1 \\
1 & +1 & -1 & +1 & +1 & -1 & -1 \\
1 & +1 & +1 & +1 & +1 & +1 & +1
\end{pmatrix},$$

$$\mathbf{X}_1^T\mathbf{X}_1 = \begin{pmatrix}
12 & 0 & 0 & 0 & -4 & 0 & 0 \\
0 & 12 & 0 & 4 & 0 & 0 & 0 \\
0 & 0 & 12 & 0 & 0 & 0 & 0 \\
0 & 4 & 0 & 12 & 0 & 0 & 0 \\
-4 & 0 & 0 & 0 & 12 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 12 & 4 \\
0 & 0 & 0 & 0 & 0 & 4 & 12
\end{pmatrix} \neq 12\mathbf{I}_7,$$

As we can see from the Tables 4.3 and 4.4, orthogonal designs may exist for some specific run size $n$ and requirements. From Deng and Tang (1999), we know that if $n$ is a multiple of 4, orthogonal designs may exist for some $\mathcal{R}$ with $q > 2$, and orthogonal designs do not exist for any $\mathcal{R}$ if $n$ is not a multiple of 4. However, as we discussed in Lemma 3 that for run size $n = N - 1$, the smallest eigenvalue is $\lambda_q = N - q$. When

$n = 12$, the smallest eigenvalue would not be larger than $N - q = 16 - 5 = 11$ since $q \geq 5$ with $k = 4$. Therefore, in this case of $k = 4$, we can not find any orthogonal design for $n = 12$ for any requirement set. $\square$

**Example 4.3**. Consider the requirement set $\mathcal{R} = \{F_1, F_2, F_3, F_4, F_1F_2, F_3F_4\}$ with $k = 4$. The AOD, AOMD, DOD and DOMD designs are computed for run size $n = 8, 9, ..., 16$. We get the following results: (1) The AOD, AOMD, DOD and DOMD designs are not unique; (2) the AOD, AOMD, DOD and DOMD designs are equivalent when $n = 8, 9, 10, 12, 13, 14, 15, 16$; there are 72 optimal designs for $n$=8, 96 for $n$=9, 576 for $n$=10, 24 for $n$=12, 96 for $n$=13, 72 for $n$=14, and 16 for $n$=15; (3) the AOD, AOMD, DOD and DOMD designs are not equivalent in the case of $n = 11$. When $n = 11$, there are 288 optimal designs for AOD, DOD and DOMD designs, and 576 AOMD designs. There are no overlap between AOMD designs and the others. Table 4.5 presents one optimal design for each run size. $\square$

**Example 4.4**. Consider the requirement set $\mathcal{R} = \{F_1, F_2, F_3, F_4, F_1F_2, F_1F_3\}$ with $k = 4$. The AOD, AOMD, DOD and DOMD designs are computed for run size $n = 8, 9, ..., 16$. We get the following results: (1) The AOD, AOMD, DOD and DOMD designs are not unique. There are 4 optimal designs for $n$=8; 32 for $n$=9; 112 for $n$=10; 224 for $n$=11; 276 for $n$=12; 208 for $n$=13; 87 for $n$=14 and 16 for $n$=15; (2) all the AOD, AOMD, DOD and DOMD designs are equivalent in this case. (c) if we switch the sign of low and high level for $F_1$, we can get the same results, which agrees with the result in the Lemma 1 in Chapter 3. Table 4.6 presents one optimal design for each run size. $\square$

**Example 4.5**. Consider Example 2.2 in Chapter 2, and the requirement set is $\mathcal{R} = \{F_1, F_2, F_3, F_1F_3\}$. Instead of running a full factorial design, we use a fractional factorial design with run size 6. There are $\binom{8}{6}$=28 choices, and 24 of them are AOD,

Table 4.5: AOD, AOMD, DOD and DOMD for Example 4.3

| run size n | optimal designs | $A(\xi_n)$ | $\mathcal{L}_A(\xi_n)$ | $D(\xi_n)^{1/q}$ | $\mathcal{L}_D(\xi_n)^{1/q}$ |
|---|---|---|---|---|---|
| 8 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ | | | | |
| | =1,2,5,8,10,11,15,16 | 1.3750 | 7.2034 | 0.1524 | 0.2236 |
| 9 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ | | | | |
| | =1,2,3,5,8,10,12,15,16 | 1.0417 | 4.0417 | 0.1281 | 0.1848 |
| 10 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ | | | | |
| | =1,2,4,5,6,9,11,14,15,16 | 0.9072 | 3.9072 | 0.1127 | 0.1626 |
| 11 | $\xi_A=\xi_D=\xi_{LD}$ | | | | |
| | =1,2,3,5,6,8,9,11,12,14,15 | 0.7750 | 3.5530 | 0.0993 | 0.1429 |
| | $\xi_{LA}$=1,2,3,5,6,8,9,11,12,13,16 | 0.7974 | 3.4237 | 0.1007 | 0.1446 |
| 12 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ | | | | |
| | =1,2,3,4,5,6,7,8,9,10,15,16 | 0.6458 | 1.6458 | 0.0876 | 0.1200 |
| 13 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ | | | | |
| | =1,2,3,4,5,6,7,9,11,12,13,14,16 | 0.5909 | 1.5909 | 0.0804 | 0.1100 |
| 14 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ | | | | |
| | =1,2,3,4,5,6,7,8,9,10,11,14,15,16 | 0.5375 | 1.5375 | 0.0738 | 0.1010 |
| 15 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ | | | | |
| | =1,2,3,4,5,6,7,8,9,10,11,12,13,14,15 | 0.4861 | 1.2639 | 0.0679 | 0.0913 |
| 16 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ | | | | |
| | =1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16 | 0.4375 | 0.4375 | 0.0625 | 0.0625 |

Table 4.6: AOD, AOMD, DOD and DOMD for Example 4.4

| run size n | optimal designs | $A(\xi_n)$ | $\mathcal{L}_A(\xi_n)$ | $D(\xi_n)^{1/q}$ | $\mathcal{L}_D(\xi_n)^{1/q}$ | $\lambda_{\min}(\mathbf{X}_1^T\mathbf{X}_1)$ |
|---|---|---|---|---|---|---|
| 8 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ =1,2,7,8,11,12,13,14 | 0.8750 | 1.8750 | 0.1250 | 0.1711 | 8.0000 |
| 9 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ =1,2,3,5,8,9,12,14,15 | 0.8167 | 1.8167 | 0.1143 | 0.15646 | 8.0000 |
| 10 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ =1,2,3,4,5,6,9,10,15,16 | 0.7589 | 1.7589 | 0.1045 | 0.1431 | 8.0000 |
| 11 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ =1,2,3,4,5,8,9,10,12,14,15 | 0.7019 | 1.7019 | 0.0957 | 0.1309 | 8.0000 |
| 12 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ =1,2,3,4,5,6,7,8,9,10,15,16 | 0.6458 | 1.6458 | 0.0876 | 0.1200 | 8.0000 |
| 13 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ =1,2,3,4,5,6,7,8,9,10,11,15,16 | 0.5909 | 1.5909 | 0.0804 | 0.1100 | 8.0000 |
| 14 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ =1,2,3,4,5,6,7,8,9,10,11,14,15,16 | 0.5375 | 1.5375 | 0.0738 | 0.1010 | 8.0000 |
| 15 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ =1,2,3,4,5,6,7,8,9,10,11,12,13,14,15 | 0.4861 | 1.2639 | 0.0679 | 0.0913 | 9.0000 |
| 16 | $\xi_A=\xi_{LA}=\xi_D=\xi_{LD}$ =1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16 | 0.4375 | 0.4375 | 0.0625 | 0.0625 | 16.0000 |

AOMD, DOD and DOMD, and they are all equivalent. Then we build the reduced model only with the data of 6 runs from the second replicate. Recall the fitted model with 16 runs (2 replicates) is:

$$\hat{y} = 1.000_{(0.203)} + 1.500_{(0.203)}x_1 + 0.875_{(0.203)}x_2 + 1.125_{(0.203)}x_3 + 0.375_{(0.203)}x_1x_3. \quad (4.1)$$

Table 4.7 presents one optimal design and the response variable from the second replicate. The fitted model based on the 6 runs in Table 4.7 is

$$\hat{y} = 1.000 + 1.125x_1 + 0.250x_2 + 0.750x_3 + 0.375x_1x_3, \quad (4.2)$$

which is similar to the fitted model in (4.1).

Table 4.7: Optimal design and response variable for Example 4.5

| optimal design | $F_1$ | $F_2$ | $F_3$ | $y$ | $\hat{y}$ |
|---|---|---|---|---|---|
| 1,2,3,4,5,6 | 10 | 200 | 25 | $-1$ | $-0.75$ |
| | 12 | 200 | 25 | 1 | 0.75 |
| | 10 | 250 | 25 | 0 | $-0.25$ |
| | 12 | 250 | 25 | 1 | 1.25 |
| | 10 | 200 | 30 | 0 | 0.00 |
| | 12 | 200 | 30 | 3 | 3.00 |
| | 10 | 250 | 30 | 1 | 0.50 |
| | 12 | 250 | 30 | 5 | 3.50 |

For each of the 24 optimal designs, we fit the reduced model and the results are shown in Figure 4.2: (a) coefficients of intercept, (b) coefficients of $F_1$, (c) coefficients of $F_2$, (d) coefficients of $F_3$, (e) coefficients of $F_1F_3$. We can conclude that they are all consistent with the coefficients of the reduced model using 16 data points. □
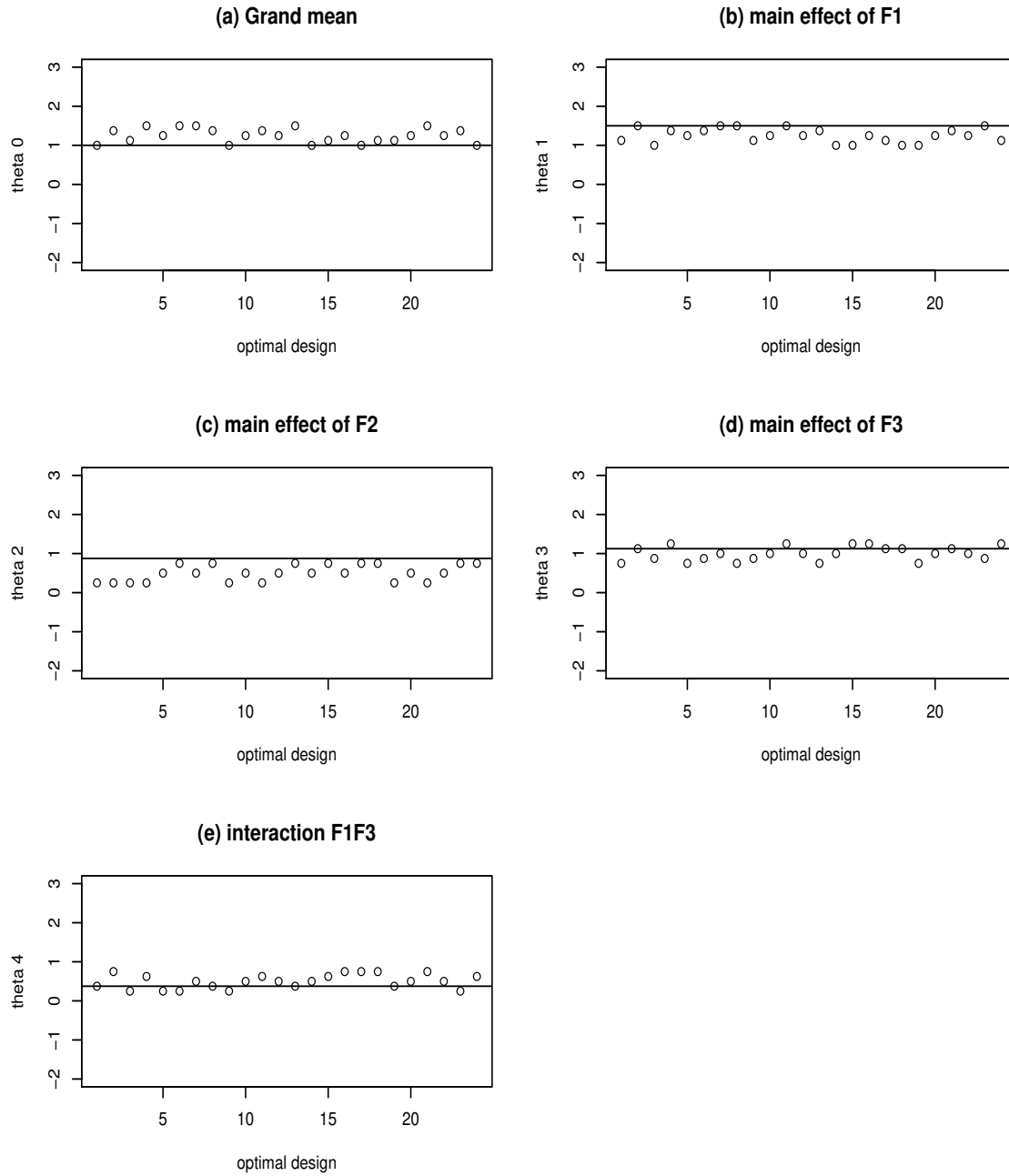
Figure 4.2: Estimated coefficients for the reduced model in Example 4.5: (a) coefficient of intercept, (b) coefficient of $F_1$, (c) coefficient of $F_2$, (d) coefficient of $F_3$, (e) coefficient of $F_1F_3$, where the horizontal lines are the estimates from the 16 data points.

## 4.4   Optimal designs from the annealing algorithm

All the results in this section are obtained from the annealing algorithm.

**Example 4.6**. Let us consider Example 4.3 again where optimal designs are computed using the complete search algorithm. Now we use the annealing algorithm to see if we can get the same optimal designs. We run the annealing algorithm with $m_0 = 5$, $T_0 = 1$, $iterT_0 = 100$ and $iter = 2000$, and some results are presented in Table 4.8. Comparing the results in Table 4.5, we notice that the optimal designs are different from Example 4.3, but their corresponding loss functions are the same. Thus the annealing algorithm is effective to find optimal designs in this example. A typical plot of the loss function for AOMD with run size $n = 11$ versus the number of iteration is given in Figure 4.3. It is clear that the loss function converges.  □

Table 4.8: AOD, AOMD, DOD and DOMD for Example 4.6

| run size n | designs | $A(\xi_n)$ | $\mathcal{L}_A(\xi_n)$ | $D(\xi_n)^{1/q}$ | $\mathcal{L}_D(\xi_n)^{1/q}$ |
|---|---|---|---|---|---|
| 8 | $\xi_A$=1,2,7,8,9,11,14,16 | 1.3750 | 7.2034 | 0.1524 | 0.2236 |
|   | $\xi_{LA}$=2,3,7,8,9,12,13,14 | 1.3750 | 7.2034 | 0.1524 | 0.2236 |
|   | $\xi_D$=1,2,5,8,10,11,15,16 | 1.3750 | 7.2034 | 0.1524 | 0.2236 |
|   | $\xi_{LD}$=1,3,5,6,11,12,14,16 | 1.3750 | 7.2034 | 0.1524 | 0.2236 |
| 9 | $\xi_A$=1,2,6,7,8,9,11,13,16 | 1.0417 | 4.0417 | 0.1281 | 0.1848 |
|   | $\xi_{LA}$=1,2,4,7,8,10,11,13,15 | 1.0417 | 4.0417 | 0.1281 | 0.1848 |
|   | $\xi_D$=1,2,6,7,9,11,12,14,16 | 1.0417 | 4.0417 | 0.1281 | 0.1848 |
|   | $\xi_{LD}$=1,2,3,5,8,10,12,15,16 | 1.0417 | 4.0417 | 0.1281 | 0.1848 |
| 10 | $\xi_A$=2,4,5,6,8,11,12,13,14,15 | 0.9072 | 3.9072 | 0.1127 | 0.1626 |
|   | $\xi_{LA}$=2,3,4,5,7,9,10,12,14,15 | 0.9072 | 3.9072 | 0.1127 | 0.1626 |
|   | $\xi_D$=1,2,5,6,8,9,11,12,14,15 | 0.9072 | 3.9072 | 0.1127 | 0.1626 |
|   | $\xi_{LD}$=1,2,5,7,8,9,10,12,14,15 | 0.9072 | 3.9072 | 0.1127 | 0.1626 |
| 11 | $\xi_A$=1,2,3,6,7,8,9,11,12,13,14 | 0.7750 | 3.5530 | 0.0993 | 0.1429 |
|   | $\xi_{LA}$=1,2,4,6,7,9,10,11,14,15,16 | 0.7974 | 3.4237 | 0.1007 | 0.1446 |
|   | $\xi_D$=1,2,3,5,6,8,10,11,12,13,16 | 0.7750 | 3.5530 | 0.0993 | 0.1429 |
|   | $\xi_{LD}$=1,2,4,5,6,10,11,12,13,15,16 | 0.7750 | 3.5530 | 0.0993 | 0.1429 |

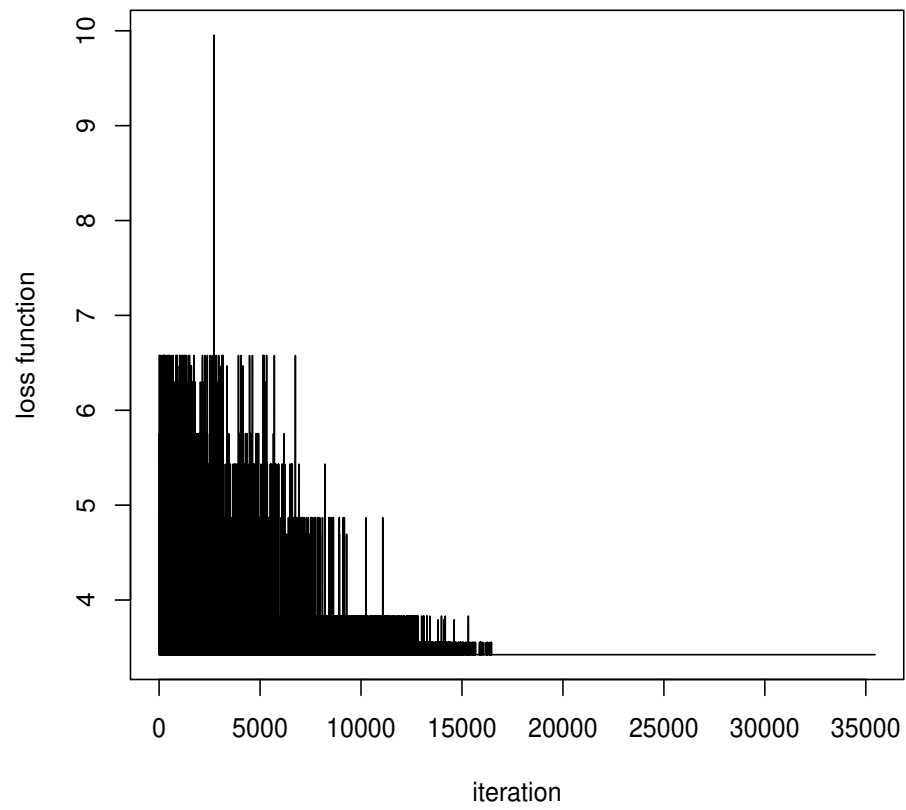**Example 4.7**. Consider the requirement set $\mathcal{R} = \{F_1, F_2, F_3, F_4, F_5, F_1F_2, F_1F_3\}$

Figure 4.3: Loss function of AOMD versus number of iteration for Example 4.6.

with $k = 5$. The AOD, AOMD, DOD and DOMD designs are computed for run size $n = 8, 9, ..., 16$. Here is the summary of the optimal designs.

(1) For $n = 8, 12, 16, 20$, the AOD, AOMD, DOD and DOMD designs are the same. For $n = 8$ and $n = 16$, the AOD, AOMD, DOD and DOMD designs are orthogonal for $\mathcal{R}$.

(2) For $n = 15$, the AOD and DOD designs are equivalent. But DOMD and AOMD are different.

(3) For $n = 19$, the AOD and DOD designs are equivalent, and the AOMD and DOMD designs are equivalent.

Table 4.9 shows some optimal designs. As we discussed before, the initial temperature $T_0$ controls the convergence rate of the solution. Figure 4.4 shows two plots of the loss function versus the iteration number for two values of the initial temperature: (a) $T_0 = 0.1$, (b) $T_0 = 1$. Both plots are set as $iterT0 = 200$ and $iter = 3000$ for run size $n = 16$ of AOMD. It is obvious that the larger $T_0 = 1$ gives higher probability to accept new designs and the loss function converges slower than the one with $T_0 = 0.1$. In Figure 4.4, in both plots, the loss functions converge to the same limit. However, a very small $T_0$ may yield a local optimal solution. □

**Example 4.8**. Consider the requirement set $\mathcal{R} = \{F_1, F_2, F_3, F_4, F_5, F_1F_2, F_1F_3, F_2F_3, F_1F_2F_3\}$ with $k = 5$. The AOD, AOMD, DOD and DOMD designs are computed for run size $n = 10, 11, 12, 15, 16, 19, 20$. We get the following results in Table 4.10.

(1) For $n = 10, 12, 16, 19, 20$, the AOD, AOMD, DOD and DOMD designs are the same.

(2) For $n = 11$, the DOD, AOMD and DOMD designs are equivalent.

Table 4.9: AOD,AOMD,DOD and DOMD for Example 4.7

| n | optimal designs | $A(\xi_n)$ | $\mathcal{L}_A(\xi_n)$ | $D(\xi_n)^{1/q}$ | $\mathcal{L}_D(\xi_n)^{1/q}$ | $\lambda_{\min}(\mathbf{X}_1^T\mathbf{X}_1)$ |
|---|---|---|---|---|---|---|
| 8 | $\xi_A$=1,7,12,14,18,24,27,29 | 1.0000 | 4.0000 | 0.1250 | 0.1869 | 8.0000 |
| | $\xi_{LA}$=3,5,10,16,20,22,25,31 | 1.0000 | 4.0000 | 0.1250 | 0.1869 | 8.0000 |
| | $\xi_D$=4,6,11,13,17,23,26,32 | 1.0000 | 4.0000 | 0.1250 | 0.1869 | 8.0000 |
| | $\xi_{LD}$=4,6,11,13,17,23,26,32 | 1.0000 | 4.0000 | 0.1250 | 0.1869 | 8.0000 |
| 12 | $\xi_A$=2,4,6,11,13,16,17,23,24,26,28,30 | 0.7292 | 3.7292 | 0.0871 | 0.1302 | 8.0000 |
| | $\xi_{LA}$=1,7,8,12,14,17,18,23,24,27,28,29 | 0.7292 | 3.7292 | 0.0871 | 0.1302 | 8.0000 |
| | $\xi_D$=1,2,7,12,14,16,20,22,24,26,27,29 | 0.7292 | 3.7292 | 0.0871 | 0.1302 | 8.0000 |
| | $\xi_{LD}$=1,2,7,12,14,16,20,22,24,26,27,29 | 0.7292 | 3.7292 | 0.0871 | 0.1302 | 8.0000 |
| 15 | $\xi_A$=2,3,5,8,9,12,14,15,17,20,22,23, 26,27,32 | 0.5625 | 3.5625 | 0.0682 | 0.1019 | 8.0000 |
| | $\xi_{LA}$=3,5,6,10,12,13,15,16,18,20,24, 25,27,30,31 | 0.5728 | 2.9314 | 0.0690 | 0.1024 | 9.5278 |
| | $\xi_D$=4,5,6,8,9,10,11,15,17,18,23,28, 29,30,32 | 0.5625 | 3.5625 | 0.0682 | 0.1019 | 8.0000 |
| | $\xi_{LD}$=1,2,3,4,7,13,14,16,21,22,24,26, 27,28,31 | 0.5625 | 3.2371 | 0.0683 | 0.1018 | 8.7085 |
| | $\xi_E$=1,3,7,8,12,13,14,18,20,21,24,25, 26,27,31 | 0.5728 | 2.9314 | 0.0690 | 0.1024 | 9.5278 |
| 16 | $\xi_A$=3,4,5,8,9,10,14,15,18,19,21,22, 25,28,31,32 | 0.5000 | 1.5000 | 0.0625 | 0.0891 | 16.0000 |
| | $\xi_{LA}$=2,3,5,6,9,12,15,16,19,20,21,24, 25,26,30,31 | 0.5000 | 1.5000 | 0.0625 | 0.0891 | 16.0000 |
| | $\xi_D$=2,3,5,8,9,12,14,15,17,20,22,23, 26,27,29,32 | 0.5000 | 1.5000 | 0.0625 | 0.0891 | 16.0000 |
| | $\xi_{LD}$=2,3,5,8,9,12,14,15,17,20,22,23, 26,27,29,32 | 0.5000 | 1.5000 | 0.0625 | 0.0891 | 16.0000 |
| 19 | $\xi_A$=3,4,5,6,9,10,13,15,16,17,18,21,23, 24,25,27,28,30,31 | 0.4363 | 1.6377 | 0.0536 | 0.0771 | 14.5359 |
| | $\xi_{LA}$=1,3,4,5,9,10,14,15,16,18,21,22, 23,24,25,26,27,28,29 | 0.4375 | 1.4375 | 0.0537 | 0.0765 | 16.0000 |
| | $\xi_D$=1,3,5,6,9,10,12,15,16,18,19,20,21, 24,25,27,29,30,31 | 0.4363 | 1.6377 | 0.0536 | 0.0771 | 14.5359 |
| | $\xi_{LD}$=2,3,5,7,8,9,12,14,15,16,18,19, 20,21,24,25,28,30,31 | 0.4375 | 1.4375 | 0.0537 | 0.0765 | 16.0000 |
| 20 | $\xi_A$=1,3,5,6,7,10,11,12,13,16,17,18,20, 23,24,25,27,29,30,31 | 0.4125 | 1.4125 | 0.0508 | 0.0723 | 16.0000 |
| | $\xi_{LA}$=1,4,6,7,8,9,11,12,13,14,15,17,18, 23,24,26,27,28,29,32 | 0.4125 | 1.4125 | 0.0508 | 0.0723 | 16.0000 |
| | $\xi_D$=1,2,3,5,7,9,12,14,15,16,19,20,21,22, 24,25,26,27,29,31 | 0.4125 | 1.4125 | 0.0508 | 0.0723 | 16.0000 |
| | $\xi_{LD}$=1,2,3,5,7,9,12,14,15,16,19,20,21, 22,24,25,26,27,29,31 | 0.4125 | 1.4125 | 0.0508 | 0.0723 | 16.0000 |

**(a)**



**(b)**
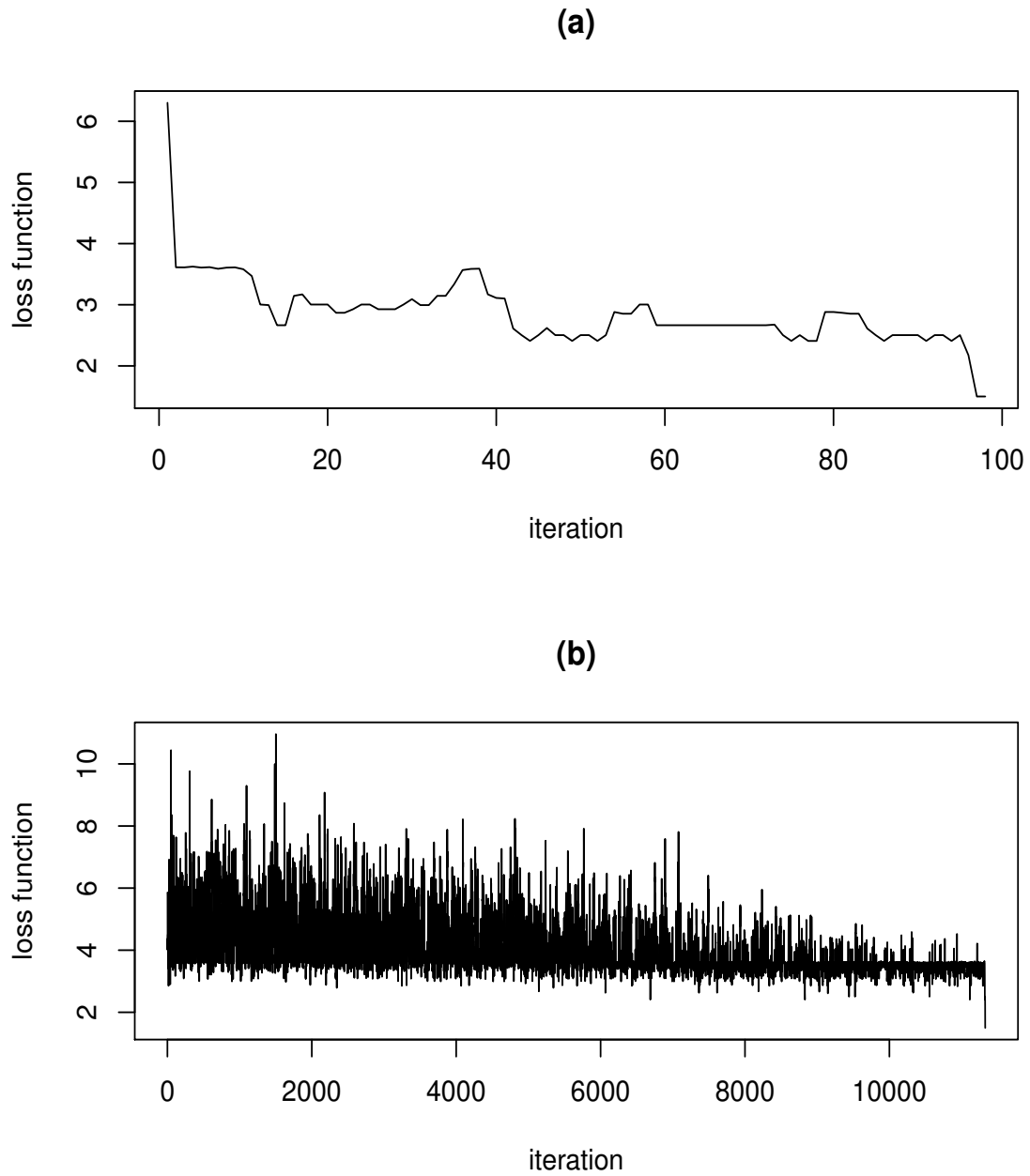


Figure 4.4: Loss function $\mathcal{L}_A(\xi_n)$ versus iteration number in Example 4.7: (a) $T_0 = 0.1$, (b) $T_0 = 1$.

(3) For $n = 15$, the AOD, DOD and DOMD designs are equivalent.

(4) For $n = 16$, the AOD, AOMD, DOD and DOMD designs are orthogonal for $\mathcal{R}$.

□

**Example 4.9**. Tang and Deng (1999) provides another criterion for nonregular fractional factorial designs. We will just use the results they gave in the paper to compare the Minimum $G_2$-aberration criterion with AOD, AOMD, DOD and DOMD criteria. The requirement set in this example is just the main effect, $\mathcal{R} = \{F_1, \cdots, F_k\}$ with $k = 5, 6, 7$. The results are shown in Table 4.11, and all the optimal designs are equivalent. in fact, they are all orthogonal for $\mathcal{R}$. In this example, we use $\xi_G$ to denote the Minimum $G_2$-aberration design. □

Table 4.10: AOD,AOMD,DOD and DOMD for Example 4.8

| n | optimal designs | $A(\xi_n)$ | $\mathcal{L}_A(\xi_n)$ | $D(\xi_n)^{1/q}$ | $\mathcal{L}_D(\xi_n)^{1/q}$ | $\lambda_{\min}(\mathbf{X}_1^T\mathbf{X}_1)$ |
|---|---|---|---|---|---|---|
| 10 | $\xi_A$=1,4,6,7,10,13,16,18,19,31 | 1.7500 | 16.7500 | 0.1250 | 0.1762 | 2.0000 |
|  | $\xi_{LA}$=6,8,12,13,17,19,21,26,30,31 | 1.7500 | 16.7500 | 0.1250 | 0.1762 | 2.0000 |
|  | $\xi_D$=1,3,8,10,13,20,21,22,27,31 | 1.7500 | 16.7500 | 0.1250 | 0.1762 | 2.0000 |
|  | $\xi_{LD}$=3,10,14,15,16,24,25,27,28,29 | 1.7500 | 16.7500 | 0.1250 | 0.1762 | 2.0000 |
| 11 | $\xi_A$=1,3,4,5,7,8,10,18,27,28,30 | 1.3438 | 11.9672 | 0.1088 | 0.1530 | 2.7530 |
|  | $\xi_{LA}$=4,5,6,7,8,10,11,18,25,28,29 | 1.3750 | 11.4981 | 0.1088 | 0.1530 | 2.8769 |
|  | $\xi_D$=3,6,10,12,13,16,17,18,21,23,27 | 1.3750 | 11.4981 | 0.1088 | 0.1530 | 2.8769 |
|  | $\xi_{LD}$=1,5,10,11,15,16,20,22,23,24,29 | 1.3750 | 11.4981 | 0.1088 | 0.1530 | 2.8769 |
| 12 | $\xi_A$=3,5,6,10,16,17,18,23,24,27,28,30 | 1.1250 | 8.1250 | 0.0947 | 0.1327 | 4.0000 |
|  | $\xi_{LA}$=1,2,6,7,11,12,16,19,20,21,26,30 | 1.1250 | 8.1250 | 0.0947 | 0.1327 | 4.0000 |
|  | $\xi_D$=2,5,8,11,14,15,17,22,23,28,29,32 | 1.1250 | 8.1250 | 0.0947 | 0.1327 | 4.0000 |
|  | $\xi_{LD}$=1,4,10,11,14,18,19,23,25,28,29,32 | 1.1250 | 8.1250 | 0.0947 | 0.1327 | 4.0000 |
| 15 | $\xi_A$=1,3,4,6,10,13,15,18,21,23,25,27,28,30,32 | 0.7240 | 4.5747 | 0.0689 | 0.0956 | 6.5969 |
|  | $\xi_{LA}$=3,6,9,12,13,15,16,17,18,20,21,23,24,27,30 | 0.7500 | 4.3625 | 0.0702 | 0.0973 | 6.9377 |
|  | $\xi_D$=1,2,5,7,11,14,16,19,22,24,25,26,28,29,31 | 0.7240 | 4.5747 | 0.0689 | 0.0956 | 6.5969 |
|  | $\xi_{LD}$=1,7,8,11,12,13,14,18,19,20,21,22,25,31,32 | 0.7240 | 4.5747 | 0.0689 | 0.0956 | 6.5969 |
| 16 | $\xi_A$=1,3,7,8,10,12,13,14,18,20,21,22,25,27,31,32 | 0.6250 | 1.6250 | 0.0625 | 0.0830 | 16.0000 |
|  | $\xi_{LA}$=1,4,5,7,10,11,14,16,18,19,22,24,25,28,29,31 | 0.6250 | 1.6250 | 0.0625 | 0.0830 | 16.0000 |
|  | $\xi_D$=2,3,4,7,9,13,14,16,17,21,22,24,26,27,28,31 | 0.6250 | 1.6250 | 0.0625 | 0.0830 | 16.0000 |
|  | $\xi_{LD}$=1,2,3,5,12,14,15,16,20,22,23,24,25,26,27,29 | 0.6250 | 1.6250 | 0.0625 | 0.0830 | 16.0000 |
| 19 | $\xi_A$=1,2,3,8,11,12,13,14,15,16,20,21,22,23,25, 26,27,29,32 | 0.5533 | 1.5533 | 0.0541 | 0.0718 | 16.0000 |
|  | $\xi_{LA}$=2,3,4,6,8,9,11,12,13,14,15,17,19,21,23, 26,28,30,32 | 0.5533 | 1.5533 | 0.0541 | 0.0718 | 16.0000 |
|  | $\xi_D$=1,4,6,8,10,11,13,15,17,18,19,21,23,24,25, 26,28,30,32 | 0.5533 | 1.5533 | 0.0541 | 0.0718 | 16.0000 |
|  | $\xi_{LD}$=1,2,3,5,6,8,10,12,13,15,18,20,21,22,23, 25,27,30,32 | 0.5533 | 1.5533 | 0.0541 | 0.0718 | 16.0000 |
| 20 | $\xi_A$=2,3,4,5,7,9,12,14,15,16,17,19,22,23,24,25, 26,27,28,29 | 0.5298 | 1.5298 | 0.0515 | 0.0684 | 16.0000 |
|  | $\xi_{LA}$=1,5,7,8,10,11,12,14,15,16,18,19,20,22,25, 26,29,30,31,32 | 0.5298 | 1.5298 | 0.0515 | 0.0684 | 16.0000 |
|  | $\xi_D$=4,5,7,8,9,10,11,14,16,17,18,19,22,23,25,28, 29,30,31,32 | 0.5298 | 1.5298 | 0.0515 | 0.0684 | 16.0000 |
|  | $\xi_{LD}$=2,3,4,6,9,10,13,15,16,17,19,21,23,24,26, 27,28,30,31,32 | 0.5298 | 1.5298 | 0.0515 | 0.0684 | 16.0000 |

Table 4.11: AOD,AOMD,DOD,DOMD and Minimum $G_2$-aberration for Example 4.9

| $k$ | optimal designs for $n = 16$ | $A(\xi_n)$ | $\mathcal{L}_A(\xi_n)$ | $D(\xi_n)^{1/q}$ | $\mathcal{L}_D(\xi_n)^{1/q}$ | $\lambda_{\min}(\mathbf{X}_1^T\mathbf{X}_1)$ |
|---|---|---|---|---|---|---|
| 5 | $\xi_A$=2,3,4,6,11,13,14,15,17,21, 23,24,25,26,28,32 | 0.3750 | 1.3750 | 0.0625 | 0.1002 | 16.0000 |
| | $\xi_{LA}$=1,3,6,8,10,12,13,15,17, 20,21,24,26,27,30,31 | 0.3750 | 1.3750 | 0.0625 | 0.1002 | 16.0000 |
| | $\xi_D$=1,3,6,8,10,11,13,16,18,20, 21,23,25,28,30,31 | 0.3750 | 1.3750 | 0.0625 | 0.1002 | 16.0000 |
| | $\xi_{LD}$=1,3,6,8,11,12,13,14,18, 20,21,23,25,26,31,32 | 0.3750 | 1.3750 | 0.0625 | 0.1002 | 16.0000 |
| | $\xi_G$=2,3,5,8,9,12,14,15,17,20, 22,23,26,27,29,32 | 0.3750 | 1.3750 | 0.0625 | 0.1002 | 16.0000 |
| 6 | $\xi_A$=1,7,10,16,18,24,25,31,36, 37,43,46,51,54,60,61 | 0.4375 | 3.4375 | 0.0625 | 0.1090 | 16.0000 |
| | $\xi_{LA}$=2,3,5,15,24,26,28,29, 38,42,43,48,49,51,56,61 | 0.4375 | 3.4375 | 0.0625 | 0.1090 | 16.0000 |
| | $\xi_D$=1,10,11,15,20,21,22,32, 34,39,40,46,51,57,60,61 | 0.4375 | 3.4375 | 0.0625 | 0.1090 | 16.0000 |
| | $\xi_{LD}$=4,6,11,13,19,21,26,32, 34,40,41,47,49,55,60,62 | 0.4375 | 3.4375 | 0.0625 | 0.1090 | 16.0000 |
| | $\xi_G$=1,4,13,16,22,23,26,27,38, 39,42,43,49,52,61,64 | 0.4375 | 3.4375 | 0.0625 | 0.1090 | 16.0000 |
| 7 | $\xi_A$=8,13,17,30,43,44,50,55,66, 71,91,92,97,110,120,125 | 0.5000 | 7.5000 | 0.0625 | 0.1129 | 16.0000 |
| | $\xi_{LA}$=4,14,19,29,38,39,58,59, 65,76,85,96,105,111,114,120 | 0.5000 | 7.5000 | 0.0625 | 0.1129 | 16.0000 |
| | $\xi_D$=3,14,20,29,39,42,54,59,66, 79,88,89,101,108,113,128 | 0.5000 | 7.5000 | 0.0625 | 0.1129 | 16.0000 |
| | $\xi_{LD}$=6,15,24,29,35,42,49,60, 65,74,84,91,104,111,117,126 | 0.5000 | 7.5000 | 0.0625 | 0.1129 | 16.0000 |
| | $\xi_G$=1,16,23,26,38,43,52,61,68, 77,86,91,103,106,113,128 | 0.5000 | 7.5000 | 0.0625 | 0.1129 | 16.0000 |

# Chapter 5
# Conclusion

We have proposed and studied the A-optimal minimax design criterion for two-level fractional factorial designs. A-optimal minimax designs are robust against the mis-specification of the requirement set, and are highly efficient comparing to A-optimal designs.

Several theoretical results are derived for A-optimal minimax designs: (1) the A-optimal minimax designs are level-permutation invariant, (2) if a design is orthogonal with respect to a requirement set, then it is A-optimal, D-optimal, E-optimal, A-optimal minimax, and D-optimal minimax design, (3) for $N - q < n \leq N - 1$, orthogonal designs for $\mathcal{R}$ don't exist, (4) lower bound of A-optimal minimax designs is derived, (5) A-optimal minimax designs are not scale invariant. Two numerical algorithms are discussed: a complete search and a simulated annealing algorithms. For small $k$ and $n$, the complete search algorithm can be applied to search for optimal designs. For moderate $k$ and $n$, the annealing algorithm is effective.

This thesis only focuses on the two-level fractional factorial designs, however the A-optimal minimax design criterion can be easily extended to mixed-level designs. The mixed-level designs include the following cases: (i) all the factors have 3 levels; (ii) some factors have 2 levels and some factors have 3 levels; (iii) all the factors or some factors have more than 3 levels.

Also, this thesis uses orthogonal regressors for the full factorial designs. If the regressors are not coded orthogonal, it is a future research topic to study A-optimal minimax and D-optimal minimax designs. Designs may be different for orthogonal

regressors and non-orthogonal regressors. The results for orthogonal regressors may not be hold for non-orthogonal regressors.

Additionally, we have used an annealing algorithm to search for optimal designs when $k$ is moderate, and it is still expensive if $k$ is large. In the future work, other efficient algorithms can be studied to search for optimal designs.

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