Selecting Baseline Two-Level Designs Using Optimality and Aberration Criteria When Some Two-Factor Interactions Are Important

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Abstract

The baseline parameterization is less commonly used in factorial designs than the orthogonal parameterization. However, the former is more natural than the latter when there exists a default or preferred setting for each factor in an experiment. The current method selects optimal baseline designs for estimating a main effect model. In this project, we consider the selection of optimal baseline designs when estimates of both main effects and some two-factor interactions are wanted. Any other potentially active effect causes bias in estimation of the important effects. To minimize the contamination of these potentially active effects, we propose a new minimum aberration criterion. Moreover, an optimality criterion is used to minimize the variances of the estimates. Finally, we develop a search algorithm for selecting optimal baseline designs based on these criteria and present some optimal designs of 16 and 20 runs for models with up to three important two-factor interactions.

Keywords: A-optimality; Baseline parameterization; Bias; D-optimality; Minimum aberration; Search algorithm

Dedication

To my parents, Xiuliang Chen and Jianhua Qi.

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Table of Contents

List of Tables

List of Figures

Chapter 1

Introduction

Factorial designs are of great practical importance in scientific and industrial investigations (Cheng, 2014, p. xv). In a full factorial design, investigators set a fixed number of levels for each factor and have a single replication of all the possible treatment combinations. Suppose that in a full factorial design, there are m factors $F_1, \ldots, F_m$ with $l_1, \ldots, l_m$ levels, respectively. Such a design is called an $l_1 \times \cdots \times l_m$ factorial design. If $l_1 = \cdots = l_m = 2$, we obtain a two-level factorial design, called a 2^m factorial design, where $N = 2^m$ is the number of runs, given by the total number of treatment combinations of m factors.

When m is large, the cost of conducting an experiment with 2^m runs is extremely high. For example, a 2^{10} factorial design requires 1024 runs. It is thus necessary to employ a design that only includes a fraction of all treatment combinations, which is called a fractional factorial (FF) design. Since FF designs allow examination of many factors with a relatively small number of runs, they are especially useful at an early stage of an experimentation (Box, Hunter, and Hunter, 1978).

In factorial experiments, we are interested in estimating main effects and interaction effects (contrasts). A main effect measures the effect of a single factor on the response averaged over all levels of other factors. A two-factor interaction (2fi) represents how two factors together affect the response. A 2fi occurs when the effect of one factor on the response depends on the levels of another factor. A full factorial design allows independent estimation of a model containing all main effects and all interactions because these contrasts form an orthogonal set. This is the orthogonal parameterization. In an FF design, some effects are aliased with each other. In other words, some effects are mixed together and cannot be distinguished from one another. Typically, we want to minimize the aliasing among the lower-order effects (like main effects and 2fi's) because the lower-order effects are more important than the higher-order effects according to the hierarchical assumption (Cheng, 2014, p. 169).

The baseline parameterization is a less common alternative to the orthogonal parameterization; however, it can be very attractive in some cases. The baseline parameterization is quite natural when there exists a default or preferred level for each factor in a design. The default level is called a baseline level and the other level is called a test level in a baseline two-level design. Because a main effect under the baseline parameterization measures the effect of a factor on the response given other factors at their baseline levels, experimenters would prefer baseline designs if they want to improve the process by changing a few factors and keeping most factors at their current levels (Li, Miller, and Tang, 2014).

In the past 30 years, many studies have been done on the selection of optimal FF designs using the minimum aberration criterion and its extensions. The minimum aberration criterion is first proposed by Fries and Hunter (1980) and is used to distinguish different designs. The idea behind the minimum aberration criterion is to sequentially minimize aliasing among effects, especially the more important lower-order effects. However, similar studies on selecting optimal FF designs under the baseline parameterization only began recently and many problems remain open. Mukerjee and Tang (2012) developed the K-aberration criterion under the baseline parameterization and proposed a method of selecting optimal baseline two-level designs under the criterion. Li, Miller, and Tang (2014) proposed an incomplete search algorithm to select best or nearly best baseline two-level designs. In both papers, main effects are of primary interest and none of the interactions are included in the fitted model. When some 2fi's are important from prior knowledge, the methods in these two papers are not appropriate, and a new method is needed.

In this project, we focus on the problem of selecting optimal baseline two-level designs when some 2fi's are important. This design problem arises naturally when there is some prior knowledge about the importance of certain 2fi's. For example, interactions between control and noise factors are usually important and should be estimated jointly with main effects in robust parameter designs (Ke and Tang, 2003). To estimate the important 2fi's, our postulated model should consist of all main effects and the important 2fi's. But in fact, we never know the true model. Any potentially active interaction not in the fitted model causes bias in estimation of main effects and the important 2fi's. Therefore, we modify the minimum K-aberration criterion proposed by Mukerjee and Tang (2012) and use the modified aberration criterion in our search algorithm to reduce the possible contamination of these active interactions. Due to the presence of important 2fi's, the universal optimality of orthogonal arrays of strength 2, shown in Mukerjee and Tang (2012), is not applicable to the new design problem. Thus, the A- or D-optimality criterion is also needed to minimize the variances of the estimates. Since two types of criteria are considered in our search algorithm, there is a trade-off between bias and variance when different orders of using the criteria lead to different optimal baseline designs.

The rest of the thesis is organized as follows. Chapter 2 introduces two types of parameterization, the optimality criteria, and the minimum K-aberration criterion with more details. Chapter 3 proposes a method of selecting optimal baseline two-level designs when some 2fi's are important. In addition, it presents a collection of optimal baseline designs of 16 and 20 runs with at most three important 2fi's. Chapter 4 summarizes this project and makes some final remarks.

Chapter 2

Definitions and Background

2.1 Two Types of Parameterization in Two-Level Fractional Factorial Designs

2.1.1 Orthogonal Parameterization

In this project, our main interest is to select optimal two-level fractional factorial (FF) designs under the baseline parameterization. Before we introduce the baseline parameterization, we recall the orthogonal parameterization first to provide some fundamental knowledge.

Consider a two-level FF design with m factors and N runs. The two levels are denoted by -1 and $+1$ for each factor. In the model matrix, corresponding to the main effect of a factor is a column vector of length N. The i^{th} component of the vector is -1 if the factor is at the low level and is $+1$ if the factor is at the high level. The low and high levels can be assigned by experimenters. For example, experimenters can regard fertilizer A as the high level and fertilizer B as the low level for a fertilizer factor in an agricultural experiment. They can also define fertilizer B as the high level and fertilizer A as the low level. This implies that the levels under the orthogonal parameterization are interchangeable. A two-factor interaction (2fi) is represented by a column vector whose i^{th} component is -1 if the corresponding two factors are at different levels (one at its high level and the other at its low level) in the i^{th} run and is $+1$ if both factors are at their high levels or low levels. The column vector of an interaction among several factors can be obtained by componentwise multiplication of the corresponding main effect vectors under the orthogonal parameterization. Table 2.1 shows the contrast coefficients for the main effects and interactions using a 2^3 design as an example, where A, B, and C are labels of the factors, called letters. A single letter, like A, B, or C, stands for a main effect, AB, AC, BC represent the

2fi's, and ABC is the three-factor interaction (3fi) in this example.

Table 2.1: The Model Matrix for a 2^3 Design under the Orthogonal Parameterization

Model matrix								**Mean response**
Intercept	**Main effects**			**2fi's**			**3fi**	
I	**A**	**B**	**C**	**AB**	**AC**	**BC**	**ABC**	$\boldsymbol{\mu}$
+1	−1	−1	−1	+1	+1	+1	−1	μ_0
+1	−1	−1	+1	+1	−1	−1	+1	μ_C
+1	−1	+1	−1	−1	+1	−1	+1	μ_B
+1	−1	+1	+1	−1	−1	+1	−1	μ_{BC}
+1	+1	−1	−1	−1	−1	+1	+1	μ_A
+1	+1	−1	+1	−1	+1	−1	−1	μ_{AC}
+1	+1	+1	−1	+1	−1	−1	−1	μ_{AB}
+1	+1	+1	+1	+1	+1	+1	+1	μ_{ABC}

The main effect of a factor is the difference in the mean response when the factor is changed from level -1 to level $+1$ averaged over the levels of all other factors. Thus, the main effects of the 2^3 design in Table 2.1 can be expressed as follows.

- Main effect of factor A is

$$\theta_A = \frac{1}{4}[(\mu_{ABC} - \mu_{BC}) + (\mu_{AB} - \mu_B) + (\mu_{AC} - \mu_C) + (\mu_A - \mu_0)].$$

- Main effect of factor B is

$$\theta_B = \frac{1}{4}[(\mu_{ABC} - \mu_{AC}) + (\mu_{AB} - \mu_A) + (\mu_{BC} - \mu_C) + (\mu_B - \mu_0)].$$

- Main effect of factor C is

$$\theta_C = \frac{1}{4}[(\mu_{ABC} - \mu_{AB}) + (\mu_{AC} - \mu_A) + (\mu_{BC} - \mu_B) + (\mu_C - \mu_0)].$$

A 2fi occurs if the main effect of one factor on the response depends on the levels of the other factor. Therefore, a 2fi represents the difference in the main effect of a factor when the other factor is changed from level -1 to level $+1$. Similarly, a 3fi shows the difference in a 2fi effect when the third factor is changed from level -1 to level $+1$. The interaction effects of the 2^3 design are shown in the following.

- Interaction between factor A and factor B is

$$\theta_{AB} = \frac{1}{4}\{[(\mu_{ABC} - \mu_{AC}) + (\mu_{AB} - \mu_A)] - [(\mu_{BC} - \mu_C) + (\mu_B - \mu_0)]\}.$$

- Interaction between factor A and factor C is

$$\theta_{AC} = \frac{1}{4}\{[(\mu_{ABC} - \mu_{AB}) + (\mu_{AC} - \mu_{A})] - [(\mu_{BC} - \mu_{B}) + (\mu_{C} - \mu_{0})]\}.$$

- Interaction between factor B and factor C is

$$\theta_{BC} = \frac{1}{4}\{[(\mu_{ABC} - \mu_{AB}) + (\mu_{BC} - \mu_{B})] - [(\mu_{AC} - \mu_{A}) + (\mu_{C} - \mu_{0})]\}.$$

- Interaction among factor A, factor B and factor C is

$$\theta_{ABC} = \frac{1}{4}\{[(\mu_{ABC} - \mu_{AB}) - (\mu_{AC} - \mu_{A})] - [(\mu_{BC} - \mu_{B}) - (\mu_{C} - \mu_{0})]\}.$$

According to the above equations, the main effects and interactions are the contrasts of the mean responses for different treatment combinations. In other words, all effects are linear combinations of the mean responses with the coefficients adding up to zero. Since these contrasts are mutually orthogonal, meaning that the sum of componentwise products of coefficients in any two contrasts is equal to zero, all effects in the 2^3 factorial design can be estimated independently under the orthogonal parameterization.

2.1.2 Baseline Parameterization

Baseline two-level designs are our main interest in the project. In a baseline design, there are a baseline level and a test level for each factor, denoted by 0 and 1, respectively. The baseline level is the default, current or preferred setting of a factor. The test level is the new setting which can possibly improve the whole process. Unlike the orthogonal parameterization, the levels under the baseline parameterization are not interchangeable.

Again, consider a two-level FF design with N runs and m factors whose levels are either 0 or 1. Under the baseline parameterization, the main effect of a factor is defined by a column vector of length N. The i^{th} component of the vector is 0 if the factor is at the baseline level in the i^{th} run and is 1 if the factor is at the test level. An interaction effect among several factors is represented by a column vector whose i^{th} component is 0 if any of the factors is at its baseline level in the i^{th} run and is 1 if the factors are all at their test levels. Like the orthogonal parameterization, the column vector of an interaction effect can be generated by componentwisely multiplying the corresponding main effect vectors under the baseline parameterization. Table 2.2 shows the model matrix of a 2^3 design under the baseline parameterization.

Table 2.2: The Model Matrix for a 2^3 Design under the Baseline Parameterization

Model matrix								**Mean response**
Intercept	**Main effects**			**2fi's**			**3fi**	
I	**A**	**B**	**C**	**AB**	**AC**	**BC**	**ABC**	$\boldsymbol{\mu}$
1	0	0	0	0	0	0	0	μ_0
1	0	0	1	0	0	0	0	μ_C
1	0	1	0	0	0	0	0	μ_B
1	0	1	1	0	0	1	0	μ_{BC}
1	1	0	0	0	0	0	0	μ_A
1	1	0	1	0	1	0	0	μ_{AC}
1	1	1	0	1	0	0	0	μ_{AB}
1	1	1	1	1	1	1	1	μ_{ABC}

Under the baseline parameterization, the main effect of a factor is the difference in the mean response when the level of the factor is changed from the baseline level to the test level while other factors remain at their baseline levels. Thus, the main effects of the 2^3 design in Table 2.2 can be expressed as follows.

- Main effect of factor A is
$$\alpha_A = \mu_A - \mu_0.$$
- Main effect of factor B is
$$\alpha_B = \mu_B - \mu_0.$$
- Main effect of factor C is
$$\alpha_C = \mu_C - \mu_0.$$

Under the baseline parameterization, a mean response for one treatment combination is written in a additive form of effects. For example, the mean response μ_{AB} is

$$\mu_{AB} = \mu_0 + \alpha_A + \alpha_B + \alpha_{AB}.$$

Then the interaction between factor A and factor B is

$$\alpha_{AB} = \mu_{AB} - \alpha_A - \alpha_B - \mu_0 = \mu_{AB} - \mu_A - \mu_B + \mu_0.$$

The other interaction effects in the 2^3 design are shown in the following.

- Interaction between factor A and factor C is
$$\alpha_{AC} = \mu_{AC} - \mu_A - \mu_C + \mu_0.$$

- Interaction between factor B and factor C is

$$\alpha_{BC} = \mu_{BC} - \mu_B - \mu_C + \mu_0.$$

- Interaction among factor A, factor B and factor C is

$$\alpha_{ABC} = \mu_{ABC} - \mu_{AB} - \mu_{AC} - \mu_{BC} + \mu_A + \mu_B + \mu_C - \mu_0.$$

Under the baseline parameterization, the main effects and interactions are still the contrasts of the mean responses for different treatment combinations. But these contrasts are not mutually orthogonal. The main difference in effects under the two types of parameterization is that the factors not involved in an effect are averaged over their levels under the orthogonal parameterization while they are fixed at their baseline levels under the baseline parameterization. The difference makes baseline designs more appropriate than orthogonal designs when experimenters want to keep most factors at their current settings and change a few factors to improve the process.

2.2 Optimality Criteria

Consider a linear model

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \tag{2.1}$$

with

$$\mathbb{E}(\boldsymbol{\epsilon}) = \mathbf{0} \text{ and } \text{cov}(\boldsymbol{\epsilon}) = \sigma^2 \boldsymbol{I}_N,$$

where $\mathbf{0}$ is a column vector of 0's with length N, $\boldsymbol{I}_N$ is an $N \times N$ identity matrix, and the common variance σ^2 is usually unknown. In addition, $\boldsymbol{Y} = (y_1, ..., y_N)^T$ is the vector of N responses, the model matrix $\boldsymbol{X}$ is an $N \times p$ matrix where the first column is a vector of 1's, $\boldsymbol{\beta} = (\beta_1, ..., \beta_p)^T$ is the vector of coefficients where the first element denotes the intercept, and $\boldsymbol{\epsilon} = (\epsilon_1, ..., \epsilon_N)^T$ is the vector of N random errors.

The least square estimator $\hat{\boldsymbol{\beta}}$ of $\boldsymbol{\beta}$ can be obtained by minimizing $||\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}||^2 = (\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})^T(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})$. If $\boldsymbol{X}^T\boldsymbol{X}$ is invertible, $\hat{\boldsymbol{\beta}} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y}$ with the covariance matrix $\text{cov}(\hat{\boldsymbol{\beta}}) = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\sigma^2$. The matrix $\boldsymbol{X}^T\boldsymbol{X}$ is called the information matrix for $\boldsymbol{\beta}$. We want a design that minimizes the covariance matrix of $\hat{\boldsymbol{\beta}}$ or equivalently minimizes the inverse of the information matrix, $(\boldsymbol{X}^T\boldsymbol{X})^{-1}$.

There are many optimality criteria aimed at minimizing $(\boldsymbol{X}^T\boldsymbol{X})^{-1}$ in some sense. The most popular are the A- and D-optimality criteria.

- A-optimality criterion minimizes the trace of $(\boldsymbol{X}^T\boldsymbol{X})^{-1}$. A design is A-optimal if it minimizes $A = \text{tr}((\boldsymbol{X}^T\boldsymbol{X})^{-1})$ among all competing designs.

- D-optimality criterion minimizes the determinant of $(\boldsymbol{X}^T\boldsymbol{X})^{-1}$. A design is D-optimal if it minimizes $D = [\det((\boldsymbol{X}^T\boldsymbol{X})^{-1})]^{1/p}$, where p is the number of coefficients in model (2.1), among all competing designs.

The A-optimality criterion is equivalent to minimizing the average variance of the estimates of coefficients. The D-optimality criterion minimizes the volume of a confidence region of coefficients because the volume is proportional to the square root of $\det((\boldsymbol{X}^T\boldsymbol{X})^{-1})$ (Atkinson and Donev, 1992). The two optimality criteria can be used under both the orthogonal and baseline parameterizations. The model matrix $\boldsymbol{X}$ can contain both main effects and interactions. In a main effect model, a design is universally optimal under the baseline parameterization if its design matrix forms a two-symbol orthogonal array of strength 2 (Mukerjee and Tang, 2012). In a two-symbol orthogonal array of strength 2, the four combinations of the two symbols occur with the same frequency for any two columns of the array. In this case, we need not worry about the design optimality. Orthogonal arrays are simply the best designs in terms of optimality.

2.3 Minimum Aberration Criterion for Baseline Designs

Mukerjee and Tang (2012) proposed the minimum K-aberration criterion for selecting optimal two-level FF designs under the baseline parameterization. In their paper, main effects are of primary interest and none of the interactions are considered in the model. In this section, we review the minimum K-aberration criterion and discuss its statistical interpretations.

Suppose the fitted model under the baseline parameterization consists of only main effects, given by

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \tag{2.2}$$

where $\boldsymbol{Y}$ is the column vector of N observations, $\boldsymbol{X}$ is the model matrix including a vector of 1's and m main effects, $\boldsymbol{\beta}$ is the column vector of coefficients with length $m+1$, and $\boldsymbol{\epsilon}$ is the vector of uncorrelated random errors with the common variance σ^2. The true model is

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \sum_{j=2}^{m} \boldsymbol{X}_j\boldsymbol{\beta}_j + \boldsymbol{\epsilon}, \tag{2.3}$$

where $\boldsymbol{X}_j$ is the model matrix for $\binom{m}{j}$ j-factor interactions, and $\boldsymbol{\beta}_j$ is the vector of the corresponding interaction effects for $j = 2, \ldots, m$. If $\boldsymbol{X}^T\boldsymbol{X}$ is invertible, then the least square estimator of $\boldsymbol{\beta}$ under the model (2.2) is

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y}, \tag{2.4}$$

which is not an unbiased estimator because the true model (2.3) also contains interactions. The expectation of $\hat{\boldsymbol{\beta}}$ is

$$\begin{aligned}\mathbb{E}(\hat{\boldsymbol{\beta}}) &= (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T(\boldsymbol{X}\boldsymbol{\beta} + \sum_{j=2}^{m}\boldsymbol{X}_j\boldsymbol{\beta}_j) \\ &= \boldsymbol{\beta} + \sum_{j=2}^{m}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{X}_j\boldsymbol{\beta}_j.\end{aligned} \tag{2.5}$$

Let $\boldsymbol{B}'_j = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{X}_j$ for $2 \leq j \leq m$. Then, the bias of $\hat{\boldsymbol{\beta}}$ is

$$\text{bias}(\hat{\boldsymbol{\beta}}, \boldsymbol{\beta}) = \sum_{j=2}^{m}\boldsymbol{B}'_j\boldsymbol{\beta}_j. \tag{2.6}$$

The first element of the vector $\boldsymbol{B}'_j\boldsymbol{\beta}_j$ represents the bias in estimation of the intercept and the remaining elements show the bias in estimation of main effects due to potentially active j-factor interactions for $2 \leq j \leq m$. Since the primary interest in Mukerjee and Tang (2012) is to estimate the main effects rather than the intercept, they removed the first row of each $\boldsymbol{B}'_j$ matrix, which determines the bias in the intercept estimate, and denoted the submatrix formed by the remaining rows as $\boldsymbol{B}_j$ for each j. Because we don't know the true values of $\boldsymbol{\beta}_j$'s, we can minimize the bias by minimizing the size of $\boldsymbol{B}_2, \ldots, \boldsymbol{B}_m$ measured by $||\boldsymbol{B}_2||^2, \ldots, ||\boldsymbol{B}_m||^2$. Let $K_j = ||\boldsymbol{B}_j||^2 = \text{trace}(\boldsymbol{B}_j^T\boldsymbol{B}_j)$ for $j \geq 2$. The minimum K-aberration criterion is defined as follows.

Definition 2.3.1. *Consider two N-run and m-factor baseline designs d_1 and d_2 formed by two-symbol orthogonal arrays of strength 2. The design d_1 has less K-aberration than d_2 if $K_s(d_1) < K_s(d_2)$, where s is the smallest positive integer so that $K_s(d_1) \neq K_s(d_2)$. A design d has the minimum K-aberration if no competing design has less K-aberration than design d.*

To sum up, Mukerjee and Tang (2012) considered the problem of selecting optimal baseline two-level designs for main effect only models in their paper. Any other active effect not in the model induces bias in estimation of the main effects measured by $K_2, \ldots, K_m$. According to the hierarchical assumption, the lower-order effects, like main effects and 2fi's, are more important than the higher-order effects (Cheng, 2014,

p. 169). Therefore, we sequentially minimize $K_2, \ldots, K_m$ to reduce the bias caused by the important lower-order effects. The minimum K-aberration criterion is a model robust criterion against the possible bias due to potentially active effects not in the fitted model.

Chapter 3

Selecting Baseline Two-Level Designs for Estimating Two-Factor Interactions

In this chapter, we focus on the problem of selecting optimal baseline two-level designs when some two-factor interactions (2fi's) are important. While the design problem of Mukerjee and Tang (2012) arises at an early stage of an investigation where the main interest is to examine the effects of many factors with a relatively small number of runs, our design problem emerges in the next stage where we have some prior knowledge about potentially important effects and want to improve the goodness of fit of our models. In this case, our postulated model consists of the intercept, all main effects, and the important 2fi's. We need to adapt the minimum K-aberration criterion to the presence of important 2fi's to minimize the bias due to potentially active interactions that are not in the model. Since the model matrix does not form a two-symbol orthogonal array of strength 2 under the baseline parameterization, we also need the A- or D-optimality criterion to minimize the variances of the estimates.

3.1 Estimation of Important Two-Factor Interactions

In this section, we adapt the minimum K-aberration criterion to the case where some 2fi's are important. The following approach is developed based on Ke and Tang (2003). The difference is that Ke and Tang (2003) considered how to select optimal regular fractional factorial (FF) designs under the orthogonal parameterization when some 2fi's are important. We consider the same problem under the baseline parameterization.

Suppose the fitted model under the baseline parameterization is composed of the intercept, all main effects, and some 2fi's, given by

$$\boldsymbol{Y} = \boldsymbol{W}\boldsymbol{\gamma} + \boldsymbol{\epsilon}, \tag{3.1}$$

where $\boldsymbol{W}$ is the model matrix with the first column of all 1's, $\boldsymbol{\gamma}$ is the vector of the intercept and the corresponding effects, and $\boldsymbol{\epsilon}$ is the vector of uncorrelated random errors with a common variance σ^2. The full model is

$$\boldsymbol{Y} = \boldsymbol{W}\boldsymbol{\gamma} + \boldsymbol{W}_2\boldsymbol{\gamma}_2 + \sum_{j=3}^{m} \boldsymbol{X}_j\boldsymbol{\beta}_j + \boldsymbol{\epsilon}, \tag{3.2}$$

where $\boldsymbol{W}_2$ is the model matrix for the rest of 2fi's, $\boldsymbol{\gamma}_2$ is the vector of the corresponding 2fi's, $\boldsymbol{X}_j$ is the model matrix for $\binom{m}{j}$ j-factor interactions, and $\boldsymbol{\beta}_j$ is the vector of the corresponding j-factor interaction effects for $j = 3, \ldots, m$. Here, m is the number of factors in the design. If $\boldsymbol{W}^T\boldsymbol{W}$ is invertible, then the estimator of $\boldsymbol{\gamma}$ under the model (3.1) is

$$\hat{\boldsymbol{\gamma}} = (\boldsymbol{W}^T\boldsymbol{W})^{-1}\boldsymbol{W}^T\boldsymbol{Y}. \tag{3.3}$$

Let $\boldsymbol{C}_2 = (\boldsymbol{W}^T\boldsymbol{W})^{-1}\boldsymbol{W}^T\boldsymbol{W}_2$ and $\boldsymbol{C}_j = (\boldsymbol{W}^T\boldsymbol{W})^{-1}\boldsymbol{W}^T\boldsymbol{X}_j$ for $3 \leq j \leq m$. Then, the bias of $\hat{\boldsymbol{\gamma}}$ under the full model (3.2) is written as

$$\text{bias}(\hat{\boldsymbol{\gamma}}, \boldsymbol{\gamma}) = \boldsymbol{C}_2\boldsymbol{\gamma}_2 + \sum_{j=3}^{m} \boldsymbol{C}_j\boldsymbol{\beta}_j. \tag{3.4}$$

The vector $\boldsymbol{C}_2\boldsymbol{\gamma}_2$ is the bias in estimation of the intercept, main effects and important 2fi's caused by other potentially active 2fi's. The vector $\boldsymbol{C}_j\boldsymbol{\beta}_j$ represents the bias due to potentially active j-factor interactions for $3 \leq j \leq m$. Since we do not know the true values of $\boldsymbol{\gamma}_2$ and $\boldsymbol{\beta}_j$'s, we guard against the bias by minimizing $||\boldsymbol{C}_2||^2, ..., ||\boldsymbol{C}_m||^2$. Let $Q_j = ||\boldsymbol{C}_j||^2 = \text{trace}(\boldsymbol{C}_j^T\boldsymbol{C}_j)$ for $2 \leq j \leq m$. We want baseline two-level designs that sequentially minimize $Q_2, ..., Q_m$. We propose a minimum Q-aberration criterion as follows.

Definition 3.1.1. *Consider two N-run and m-factor baseline designs d_1 and d_2 whose model matrices contain the same set of two-factor interactions. The design d_1 has less Q-aberration than d_2 if $Q_s(d_1) < Q_s(d_2)$, where s is the smallest positive integer so that $Q_s(d_1) \neq Q_s(d_2)$. A design d has the minimum Q-aberration if no competing design has less Q-aberration than design d.*

3.2 Different Structures of Two-Factor Interactions

Both the minimum Q-aberration criterion and the optimality criteria depend on the fitted model. Thus, we need to specify which 2fi's are included in the fitted model before we use the criteria. Let m denote the number of factors in a design. Then, there are $\binom{m}{2}$ possible 2fi's. Any subset of these 2fi's can be included in the fitted model. Altogether, there are 2^V subsets (including the special case of no 2fi in the model), where $V = \binom{m}{2}$. Even for a small m, 2^V is a huge number and it is nearly impossible to consider all cases. So for simplicity, we only consider cases of up to three 2fi's in the fitted model.

Even for a small number of 2fi's in the model, the structures of 2fi's can be very different. For example, when there are two 2fi's in the model, the 2fi's can be in the form of AB and AC or AB and CD. In other words, the two 2fi's can have a factor in common or have totally different factors. The more 2fi's in the fitted model, the more possible structures of 2fi's. Ke and Tang (2003) used the graph theory to represent different 2fi structures. Let a vertex denote a factor and an edge represent a 2fi. Then, the following three figures show the 2fi structures for models containing one, two and three 2fi's, respectively (Ke and Tang, 2003).

Figure 3.1: Graph for One Two-Factor Interaction.

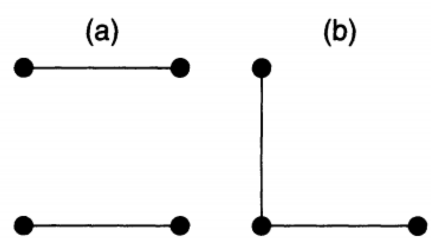

Figure 3.2: Graphs for Two Two-Factor Interactions.

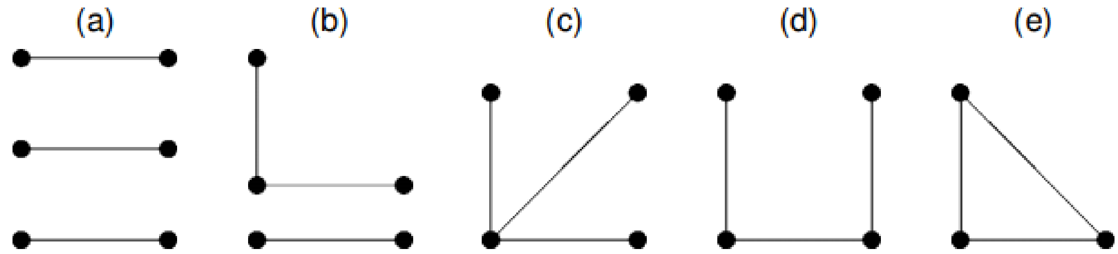

Figure 3.3: Graphs for Three Two-Factor Interactions.

3.3 Isomorphism for Baseline Designs

In this section, we introduce the definition of isomorphic designs under the baseline parameterization. If two baseline designs are isomorphic, they have the same properties, such as the same optimality and Q-aberration, and thus can be regarded as the same design. We can reduce computational cost by searching for optimal designs from a complete set of nonisomorphic designs.

Under the orthogonal parameterization, two designs are defined to be isomorphic if one design can be obtained from the other by permuting rows and columns, interchanging the signs of two levels, or a combination of these operations (Ke and Tang, 2003). The definition of isomorphism is slightly different under the baseline parameterization because the levels of baseline designs are not interchangeable. To distinguish the two types of isomorphism, we call isomorphism under the orthogonal parameterization combinatorial isomorphism. The definition of isomorphic designs under the baseline parameterization is in the following (Mukerjee and Tang, 2012).

Definition 3.3.1. *Two baseline designs are isomorphic if one design can be obtained from the other by permuting rows and columns.*

These two definitions suggest a relation between nonisomorphic designs and combinatorially nonisomorphic designs. That is, given a complete set of combinatorially nonisomorphic designs, we can generate a complete set of nonisomorphic designs by interchanging the levels of one or more columns for each combinatorially nonisomorphic design. The detailed algorithm is developed by Mukerjee and Tang (2012) and is shown as follows.

1. Choose a design from the complete set of combinatorially nonisomorphic designs. For each possible subset of its columns, generate a new design by interchanging

the levels of the columns in the subset. If there are m factors in the original design, there are 2^m designs generated in this step (including the original design).

2. Repeat step 1 for all the combinatorially nonisomorphic designs.

3. All the designs generated in steps 1 and 2 form a complete set of nonisomorphic designs. If there are q combinatorially nonisomorphic designs, then there are $2^m q$ designs in the complete set of nonisomorphic designs.

Note that there are possibly some isomorphic designs among the $2^m q$ designs. When m is small, these isomorphic designs are not a big concern in terms of added computing time.

3.4 Search for Optimal Baseline Designs

In this section, we show how to select optimal baseline designs using the A-optimality criterion and the minimum Q-aberration criterion. Before discussing the search algorithm, we need to clarify what an optimal baseline design is. Ideally, the optimal designs have the smallest A value (A-best), and the minimum Q-aberration among all the competing baseline designs. Such designs can be represented by the intersection in Figure 3.4(a), where the order of using the A-optimality criterion and the minimum Q-aberration criterion does not affect the selection results. No matter which set we start with, we eventually obtain the intersection in Figure 3.4(a). However, the intersection between the set of the A-best designs and the set of the minimum Q-aberration designs may be empty as in case (b), where different orders of using the two criteria can lead to different optimal designs. In case (b), we face a trade-off between bias and variance. If a large bias is a bigger concern than a large variance, we can first use the minimum Q-aberration criterion to minimize the bias and then select the A-best designs from the minimum Q-aberration designs; otherwise, we first use the A-optimality criterion. Mukerjee and Tang (2012) suggested using the second approach because the number of potentially active 2fi's is usually not large and the higher-order effects are more likely to be negligible than the lower-order effects. The above arguments equally apply if the A-optimality criterion is replaced by the D-optimality criterion.

In our search algorithm, we use the A-optimality criterion first and then select the minimum Q-aberration designs from the A-best baseline designs. Let N denote the number of runs, m be the number of factors, and f represent the number of 2fi's in a baseline two-level design. Then, our search algorithm is shown as follows.

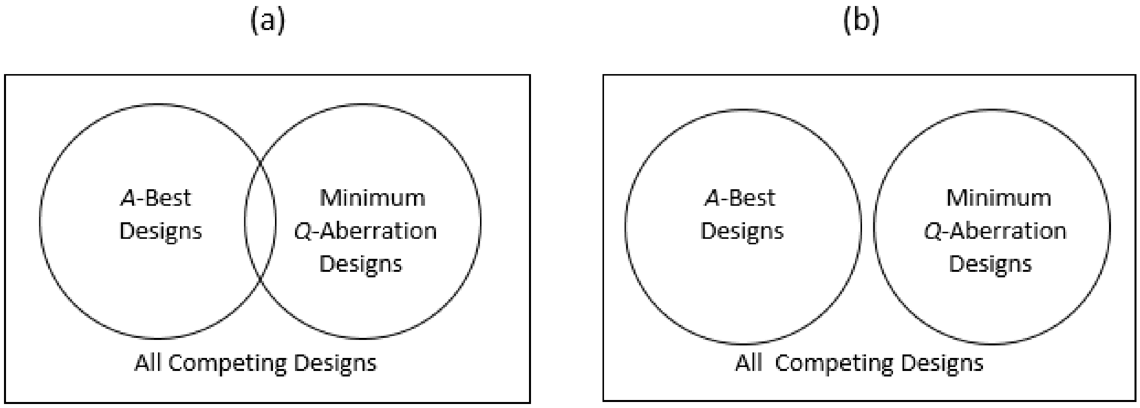

Figure 3.4: Relations between A-Best Designs and Minimum Q-Aberration Designs

1. For a given N and m, find all combinatorially nonisomorphic two-level FF designs using levels 0 and 1. Suppose there are q such designs.

2. For each of the q designs, generate a complete set of nonisomorphic designs by interchanging the levels of one or more columns (details in Section 3.3). A total of $2^m q$ designs are obtained in this step.

3. For a given f, each of the $2^m q$ designs is a design matrix for main effects and we then construct all possible model matrices for all the main effects and f 2fi's. To obtain the f 2fi's, consider all possible 2fi structures and then assign different factors to those vertices in each structure. For example, when $f = 2$, there are two 2fi structures (Figure 3.2 in Section 3.2), $\binom{m}{2}\binom{m-2}{2}/2$ ways to assign factors in Figure 3.2(a), and $\binom{m}{1}\binom{m-1}{2}$ ways to assign factors in Figure 3.2(b). Suppose there are g different 2fi structures and c_i possible ways to assign factors in the i^{th} structure for $i = 1, \ldots, g$. Then, in the i^{th} 2fi structure, there are $2^m qc_i$ model matrices for $i = 1, \ldots, g$.

4. For each 2fi structure, compute the values of A, $Q_2, \ldots, Q_m$ for each of the $2^m qc_i$ model matrices and find the optimal baseline two-level designs that sequentially minimize A, $Q_2, \ldots, Q_m$.

Here, we can also use the D-optimality criterion in the same way, and the results may not agree with those given by the A-optimality criterion. Also, we can easily switch the order of using the two types of criteria by minimizing $Q_2, \ldots, Q_m$, A sequentially.

3.5 Search Results

3.5.1 Baseline Designs of 16 Runs

Tables 3.1, 3.2, and 3.3 present 16-run optimal baseline two-level designs for models containing one, two, and three 2fi's, respectively. In these tables, "m" represents the number of factors. The "model" refers to the 2fi structures shown in Figures 3.1, 3.2, and 3.3 of Section 3.2. For example, if the "model" is 2(b) for an optimal design, the 2fi structure for the design corresponds to graph (b) in the second figure of Section 3.2. The "parent design" stands for the combinatorially nonisomorphic designs from which optimal designs are generated. These parent designs are originally from Chen, Sun, and Wu (1993), who presented a complete list of nonisomorphic regular two-level FF designs of 16 runs under the orthogonal parameterization. To generate baseline designs from the orthogonal designs, we can simply replace level -1 with level 0 in the design matrices. The details of the parent designs are shown in Table 3.4, and the columns listed in Table 3.4 are given in Table 3.5. The "2fi's" show which 2fi's are included in the models. The "relabeling" lists the columns whose levels are interchanged in step 2 of our algorithm. Again, the entries under "2fi's" and "relabeling" refer to the columns in Table 3.5. The last three columns in Tables 3.1, 3.2, and 3.3, respectively, provide the D values, A values, and the first three Q values for optimal designs.

In Table 3.1, it is interesting to note that the D values are the same for all optimal designs no matter how many factors are in the designs. In Tables 3.2 and 3.3, the D values and A values are the same for a given m and a given number of 2fi's regardless of their 2fi structures. Furthermore, all competing designs are equally efficient for each case considered in the three tables. Therefore, the set of the minimum Q-aberration designs is a subset of the set of the A-best (or D-best) designs, and the 16-run optimal designs are actually the minimum Q-aberration designs, which is a special case of Figure 3.4(a) in Section 3.4. For these optimal designs, the labels of their parent designs often do not end up with ".1", which implies that their parent designs are usually not the minimum aberration designs.

Table 3.1: Optimal Baseline Designs of 16 Runs for the Models Containing One 2fi

m	Parent design	2fi	Relabeling	D value	A value	(Q_2, Q_3, Q_4)
5	5-1.2	(1, 8)	1	0.25	3.19	(5.06, 2.8, 0.55)
6	6-2.2	(2, 4)	1	0.25	3.5	(8.44, 6.08, 1.81)
7	7-3.2	(1, 8)	1, 8	0.25	3.81	(12.38, 11.33, 4.97)
8	8-4.2	(1, 14)	1, 14	0.25	4.13	(16.88, 19.12, 11.5)
9	9-5.3	(1, 14)	1, 6	0.25	4.44	(24.5, 33.16, 24.09)
10	10-6.2	(2, 13)	2, 5, 9	0.25	4.75	(32.69, 49.7, 39.75)
11	11-7.1	(1, 14)	3, 4, 8	0.25	5.06	(41.44, 72.08, 67.34)
12	12-8.2	(4, 9)	1, 2, 3, 12	0.25	5.38	(51.88, 100.44, 102.38)
13	13-9.1	(2, 12)	1, 2, 3, 12, 13	0.25	5.69	(62.88, 135.88, 156.14)
14	14-10.1	(1, 14)	1, 2, 3, 12, 13, 14	0.25	6	(75, 179, 228.5)

Table 3.2: Optimal Baseline Designs of 16 Runs for the Models Containing Two 2fi's

m	Model	Parent design	2fi's	Relabeling	D value	A value	(Q_2, Q_3, Q_4)
5	2(a)	5-1.1	(1, 2) (4, 8)	None	0.30	4.75	(4.5, 3.69, 0.78)
	2(b)	5-1.2	(1, 8) (2, 8)	1	0.30	4.75	(4.5, 3.19, 0.72)
6	2(a)	6-2.2	(2, 4) (3, 8)	1	0.29	5.06	(7.88, 7.27, 2.45)
	2(b)	6-2.2	(2, 4) (3, 4)	1	0.29	5.06	(7.88, 7.05, 2.36)
7	2(a)	7-3.3	(4, 8) (5, 10)	1, 8	0.29	5.38	(12.38, 13.25, 6.19)
	2(b)	7-3.2	(1, 8) (1, 14)	1, 8	0.29	5.38	(11.81, 13.5, 6.66)
8	2(a)	8-4.5	(2, 8) (6, 9)	1, 6	0.28	5.69	(18.88, 23.56, 13.31)
	2(b)	8-4.5	(6, 8) (6, 9)	1, 6	0.28	5.69	(17.44, 22.23, 13.95)
9	2(a)	9-5.4	(4, 9) (6, 8)	1, 2, 3	0.28	6	(25.94, 38, 26.64)
	2(b)	9-5.4	(4, 9) (4, 10)	1, 2, 3	0.28	6	(25.94, 37.75, 26.36)
10	2(a)	10-6.2	(2, 13) (4, 10)	2, 5, 9	0.28	6.31	(35, 59.61, 50.29)
	2(b)	10-6.2	(2, 13) (3, 13)	2, 5, 9	0.28	6.31	(35, 59.23, 49.39)
11	2(a)	11-7.3	(4, 8) (5, 10)	1, 2, 3	0.28	6.63	(45.75, 86, 79.62)
	2(b)	11-7.3	(4, 8) (4, 9)	1, 2, 3	0.28	6.63	(45.75, 86, 80.12)
12	2(a)	12-8.2	(4, 9) (6, 8)	1, 2, 3, 12	0.27	6.94	(57.06, 121.55, 129.09)
	2(b)	12-8.2	(4, 9) (4, 10)	1, 2, 3, 12	0.27	6.94	(57.06, 121.42, 128.84)
13	2(a)	13-9.1	(2, 12) (4, 11)	1, 2, 3, 12, 13	0.27	7.25	(69.5, 164.5, 196.81)
	2(b)	13-9.1	(2, 12) (2, 13)	1, 2, 3, 12, 13	0.27	7.25	(69.5, 164.5, 196.94)

Table 3.3: Optimal Baseline Designs of 16 Runs for the Models Containing Three 2fi's

m	Model	Parent design	2fi's	Relabeling	D value	A value	(Q_2, Q_3, Q_4)
5	3(a)	-	-	-	-	-	-
	3(b)	5-1.1	(1, 2) (1, 4) (8, 15)	None	0.34	6.31	(3.94, 4.47, 1.04)
	3(c)	5-1.2	(1, 8) (2, 8) (4, 8)	1	0.34	6.31	(3.94, 3.73, 0.89)
	3(d)	5-1.1	(1, 2) (1, 4) (2, 8)	None	0.34	6.31	(3.94, 4.56, 1.19)
	3(e)	5-1.1	(1, 2) (1, 4) (2, 4)	None	0.34	6.31	(3.94, 4.66, 1.35)
6	3(a)	6-2.3	(1, 4) (2, 8) (3, 12)	1, 4	0.33	6.63	(7.88, 8.62, 2.95)
	3(b)	6-2.2	(2, 4) (2, 8) (3, 13)	1	0.33	6.63	(7.31, 8.61, 3.2)
	3(c)	6-2.2	(2, 4) (2, 8) (2, 13)	1	0.33	6.63	(7.31, 8.8, 3.33)
	3(d)	6-2.2	(2, 4) (2, 8) (3, 4)	1	0.33	6.63	(7.31, 8.39, 3.11)
	3(e)	6-2.2	(2, 4) (2, 8) (4, 8)	2	0.33	6.63	(8.75, 9.91, 3.83)
7	3(a)	7-3.2	(1, 8) (2, 5) (4, 14)	1	0.32	6.94	(14.12, 18, 8.91)
	3(b)	7-3.2	(1, 8) (1, 14) (2, 5)	1, 8	0.32	6.94	(12.69, 16.7, 8.48)
	3(c)	7-3.5	(1, 8) (2, 8) (4, 8)	1, 6	0.32	6.94	(12.38, 13.8, 5.27)
	3(d)	7-3.3	(4, 8) (4, 10) (5, 8)	1, 8	0.32	6.94	(11.81, 14.75, 7.44)
	3(e)	7-3.2	(1, 8) (1, 14) (8, 14)	1	0.32	6.94	(14.12, 18.64, 9.92)
8	3(a)	8-4.3	(1, 10) (2, 5) (3, 12)	1, 8	0.31	7.25	(20.62, 29.31, 17.53)
	3(b)	8-4.5	(2, 8) (5, 9) (6, 8)	1, 6	0.31	7.25	(19.75, 27.25, 15.48)
	3(c)	8-4.6	(1, 8) (2, 8) (4, 8)	1, 2, 3	0.31	7.25	(18, 23.12, 11.31)
	3(d)	8-4.5	(2, 8) (6, 8) (6, 9)	1, 6	0.31	7.25	(18.31, 25.92, 16.09)
	3(e)	8-4.3	(1, 10) (1, 12) (10, 12)	1, 8	0.31	7.25	(22.06, 32.06, 19.44)
9	3(a)	9-5.4	(4, 9) (5, 10) (6, 8)	1, 2, 3	0.31	7.56	(26.81, 43.77, 32.45)
	3(b)	9-5.5	(2, 8) (4, 8) (6, 9)	1, 2, 3	0.31	7.56	(27.38, 42.75, 28.75)
	3(c)	9-5.5	(2, 8) (4, 8) (6, 8)	1, 2, 3	0.31	7.56	(27.38, 42.25, 28)
	3(d)	9-5.4	(4, 9) (4, 10) (5, 10)	1, 2, 3	0.31	7.56	(26.81, 43.27, 31.89)
	3(e)	9-5.2	(1, 8) (1, 15) (8, 15)	1, 8, 15	0.31	7.56	(30.56, 51.09, 38.1)
10	3(a)	10-6.4	(4, 8) (5, 10) (7, 9)	1, 2, 3	0.30	7.88	(37.88, 68.33, 56.28)
	3(b)	10-6.4	(4, 8) (4, 9) (5, 10)	1, 2, 3	0.30	7.88	(37.88, 68.2, 56.28)
	3(c)	10-6.4	(4, 8) (4, 9) (4, 10)	1, 2, 3	0.30	7.88	(37.88, 67.95, 56.28)
	3(d)	10-6.4	(4, 8) (4, 9) (6, 8)	1, 2, 3	0.30	7.88	(37.88, 68.08, 56.28)
	3(e)	10-6.2	(6, 10) (6, 13) (10, 13)	2, 5, 9	0.30	7.88	(41.62, 76.97, 63.8)
11	3(a)	11-7.3	(4, 8) (5, 10) (6, 11)	1, 2, 3	0.30	8.19	(49.5, 100.25, 95.38)
	3(b)	11-7.3	(4, 8) (4, 9) (5, 10)	1, 2, 3	0.30	8.19	(49.5, 100.25, 95.88)
	3(c)	11-7.3	(4, 8) (4, 9) (4, 10)	1, 2, 3	0.30	8.19	(49.5, 100.25, 96.88)
	3(d)	11-7.3	(4, 8) (4, 9) (6, 8)	1, 2, 3	0.30	8.19	(49.5, 100.25, 96.38)
	3(e)	11-7.1	(1, 6) (1, 10) (6, 10)	3, 4, 8	0.30	8.19	(53.25, 112.45, 111.03)
12	3(a)	12-8.2	(4, 9) (5, 10) (6, 8)	1, 2, 3, 12	0.30	8.5	(62.25, 142.62, 155.75)
	3(b)	12-8.2	(4, 9) (4, 10) (7, 8)	1, 2, 3, 12	0.30	8.5	(62.25, 142.5, 155.5)
	3(c)	12-8.2	(4, 9) (4, 10) (4, 11)	1, 2, 3, 12	0.30	8.5	(62.25, 142.25, 155)
	3(d)	12-8.2	(4, 9) (4, 10) (5, 10)	1, 2, 3, 12	0.30	8.5	(62.25, 142.38, 155.25)
	3(e)	12-8.1	(1, 6) (1, 10) (6, 10)	1, 6, 10, 13	0.30	8.5	(66, 156, 177)

Note: "-" means that there is no such model for the given m.

Table 3.4: The Parent Designs of 16 Runs

m	Parent design	Additional columns
5	5-1.1	15
	5-1.2	7
6	6-2.2	3, 13
	6-2.3	3, 12
7	7-3.2	3, 5, 14
	7-3.3	3, 5, 10
	7-3.5	3, 5, 6
8	8-4.2	3, 5, 9, 14
	8-4.3	3, 5, 10, 12
	8-4.5	3, 5, 6, 9
	8-4.6	3, 5, 6, 7
9	9-5.2	3, 5, 10, 12, 15
	9-5.3	3, 5, 6, 9, 14
	9-5.4	3, 5, 6, 9, 10
	9-5.5	3, 5, 6, 7, 9
10	10-6.2	3, 5, 6, 9, 10, 13
	10-6.4	3, 5, 6, 7, 9, 10
11	11-7.1	3, 5, 6, 9, 10, 13, 14
	11-7.3	3, 5, 6, 7, 9, 10, 11
12	12-8.1	3, 5, 6, 9, 10, 13, 14, 15
	12-8.2	3, 5, 6, 7, 9, 10, 11, 12
13	13-9.1	3, 5, 6, 7, 9, 10, 11, 12, 13
14	14-10.1	3, 5, 6, 7, 9, 10, 11, 12, 13, 14

Note: Each design includes four independent columns 1, 2, 4, 8 and the additional columns.

Table 3.5: The Saturated Design of 16 Runs

1	**2**	3	**4**	5	6	7	**8**	9	10	11	12	13	14	15
0	**0**	1	**0**	1	1	0	**0**	1	1	0	1	0	0	1
0	**0**	1	**0**	1	1	0	**1**	0	0	1	0	1	1	0
0	**0**	1	**1**	0	0	1	**0**	1	1	0	0	1	1	0
0	**0**	1	**1**	0	0	1	**1**	0	0	1	1	0	0	1
0	**1**	0	**0**	1	0	1	**0**	1	0	1	1	0	1	0
0	**1**	0	**0**	1	0	1	**1**	0	1	0	0	1	0	1
0	**1**	0	**1**	0	1	0	**0**	1	0	1	0	1	0	1
0	**1**	0	**1**	0	1	0	**1**	0	1	0	1	0	1	0
1	**0**	0	**0**	0	1	1	**0**	0	1	1	1	1	0	0
1	**0**	0	**0**	0	1	1	**1**	1	0	0	0	0	1	1
1	**0**	0	**1**	1	0	0	**0**	0	1	1	0	0	1	1
1	**0**	0	**1**	1	0	0	**1**	1	0	0	1	1	0	0
1	**1**	1	**0**	0	0	0	**0**	0	0	0	1	1	1	1
1	**1**	1	**0**	0	0	0	**1**	1	1	1	0	0	0	0
1	**1**	1	**1**	1	1	1	**0**	0	0	0	0	0	0	0
1	**1**	1	**1**	1	1	1	**1**	1	1	1	1	1	1	1

Note: Columns 1, 2, 4, and 8 are independent columns.

3.5.2 Baseline Designs of 20 Runs

Tables 3.6, 3.7 and 3.8 show the optimal baseline two-level designs of 20 runs. We only consider optimal designs with $m = 4, 5, 6, 7$, as the number of combinatorially nonisomorphic designs becomes exceedingly large for $m \geq 8$. According to a previous study (Sun, Li, and Ye, 2008), there are 3, 11, 75, and 474 combinatorially nonisomorphic designs for $m = 4, 5, 6, 7$, respectively. To identify these designs, we label them sequentially according to the order they occur in each complete set of combinatorially nonisomorphic designs. In Tables 3.6, 3.7 and 3.8, the entries under "parent design" refer to these design labels. For example, when $m = 4$, the parent design of the optimal design in Table 3.6 is the first design (design No.1) in the complete set. The entries under "2fi's" and "relabeling" refer to the column indices in the corresponding parent designs. For the convenience of the reader, we provide in Appendix A a full display of the parent designs of 20 runs.

For each case in Tables 3.6, 3.7 and 3.8, the corresponding competing designs are not equally efficient. Thus, the optimal designs are the minimum Q-aberration designs selected from the A-best designs, which corresponds to the case of Figure 3.4(b). If we use the D-optimality criterion in our algorithm, we get the same results except three cases in Table 3.8: $m = 5$, model=3(b); $m = 6$, model=3(a); $m = 7$, model=3(d). These three designs are included in Table 3.8, which are identified with a "*".

Table 3.6: Optimal Baseline Designs of 20 Runs for the Model Containing One 2fi

m	Parent design	2fi	Relabeling	D value	A value	(Q_2, Q_3, Q_4)
4	1	(1, 2)	1, 2, 4	0.20	2.39	(2.78, 1.07, 0)
5	8	(3, 5)	None	0.20	2.7	(5.24, 2.62, 0.26)
6	70	(2, 5)	1, 2, 5	0.20	3.02	(8.56, 5.78, 1.27)
7	471	(4, 6)	1, 3, 4, 6, 7	0.21	3.35	(12.55, 11.26, 4.22)

Table 3.7: Optimal Baseline Designs of 20 Runs for the Models Containing Two 2fi's

m	Model	Parent design	2fi's	Relabeling	D value	A value	(Q_2, Q_3, Q_4)
4	2(a)	1	(1, 2) (3, 4)	1, 2, 4	0.25	3.80	(2.37, 1.22, 0)
	2(b)	1	(1, 2) (1, 3)	1, 2, 4	0.25	3.75	(2.30, 1.50, 0)
5	2(a)	10	(1, 2) (3, 5)	2, 3, 5	0.25	4.16	(5.21, 3.57, 0.29)
	2(b)	8	(1, 5) (3, 5)	None	0.25	4.13	(4.96, 3.10, 0.34)
6	2(a)	67	(1, 5) (4, 6)	2, 3, 4, 5	0.24	4.53	(8.83, 7.74, 2.34)
	2(b)	47	(2, 6) (3, 6)	1, 2, 3, 5, 6	0.24	4.52	(8.62, 7.02, 1.93)
7	2(a)	403	(1, 4) (3, 7)	2, 3, 4, 6, 7	0.24	4.94	(13.42, 14.13, 6.20)
	2(b)	451	(1, 5) (2, 5)	3, 4, 5, 7	0.24	4.92	(13.23, 15.33, 7.83)

Table 3.8: Optimal Baseline Designs of 20 Runs for the Models Containing Three 2fi's

m	Model	Parent design	2fi's	Relabeling	D value	A value	(Q_2, Q_3, Q_4)
4	3(a)	-	-	-	-	-	-
	3(b)	-	-	-	-	-	-
	3(c)	1	(1, 2) (1, 3) (1, 4)	1, 2, 4	0.29	5.13	(1.8, 1.98, 0)
	3(d)	1	(1, 2) (1, 3) (2, 4)	1, 2, 4	0.29	5.19	(1.85, 1.69, 0)
	3(e)	1	(1, 2) (1, 3) (2, 3)	None	0.29	5.11	(2.14, 2.18, 0.31)
5	3(a)	-	-	-	-	-	-
	3(b)	5	(1, 4) (2, 5) (3, 5)	1, 2, 5	0.29	5.68	(4.88, 4.35, 0.70)
	3(b)*	10	(1, 2) (3, 5) (4, 5)	1, 4, 5	0.29	5.71	(4.84, 4.71, 0.54)
	3(c)	8	(1, 5) (2, 5) (3, 5)	1, 2, 5	0.28	5.58	(4.75, 4.67, 0.88)
	3(d)	10	(1, 2) (1, 4) (4, 5)	1, 4, 5	0.29	5.62	(4.84, 4.21, 0.36)
	3(e)	10	(1, 2) (1, 5) (2, 5)	None	0.28	5.55	(5.12, 4.33, 0.89)
6	3(a)	46	(1, 6) (2, 5) (3, 4)	1, 3	0.28	6.13	(8.75, 8.16, 2.37)
	3(a)*	57	(1, 4) (2, 5) (3, 6)	1, 4, 6	0.28	6.20	(8.71, 9.56, 3.35)
	3(b)	46	(1, 6) (3, 4) (3, 5)	1, 3, 5	0.28	6.09	(8.92, 9.85, 3.31)
	3(c)	69	(1, 5) (4, 5) (5, 6)	None	0.28	6.03	(8.67, 9.60, 2.92)
	3(d)	67	(1, 5) (4, 6) (5, 6)	2, 3, 4, 5	0.28	6.05	(8.71, 9.29, 3.04)
	3(e)	58	(4, 5) (4, 6) (5, 6)	4, 5	0.28	5.99	(9.08, 10.35, 6.66)
7	3(a)	429	(2, 7) (3, 6) (4, 5)	2	0.27	6.55	(14.07, 16.70, 7.32)
	3(b)	334	(1, 5) (2, 6) (5, 7)	1, 2, 4, 5, 7	0.27	6.53	(13.91, 17.15, 8.00)
	3(c)	430	(1, 5) (1, 6) (1, 7)	1, 7	0.27	6.48	(13.89, 15.91, 6.82)
	3(d)	90	(1, 7) (3, 6) (3, 7)	2, 4, 6, 7	0.27	6.53	(13.97, 16.03, 6.16)
	3(d)*	429	(3, 5) (3, 6) (4, 5)	1, 2, 4	0.27	6.55	(13.68, 17.57, 7.90)
	3(e)	425	(4, 6) (4, 7) (6, 7)	5, 6, 7	0.27	6.48	(14.27, 16.33, 6.52)

Note: 1. "-" means that there is no such model for the given m.
2. The designs designated by "*" are selected using the D-criterion instead of the A-criterion.

3.6 An Example

In this section, we use an example to explain how to use the tables of optimal designs in Section 3.5. Suppose that experimenters want to improve the recipe of a cake and they study eight factors including baking time, baking temperature, the number of eggs, and the amounts of baking powder, flour, sugar, milk and butter. For each factor, there are two levels; one is the original setting and the other is the new setting. The experimenters conduct an experiment in 16 runs. According to the prior knowledge, the interactions between baking temperature and baking time and between the amount of milk and baking time are important and should be estimated. Since there are two 2fi's in the model with 16 runs and 8 factors, we need to look at the cases with m=8 in Table 3.2 of Section 3.5. Because the two important 2fi's have one common factor, its 2fi structure is 2(b) corresponding to Figure 3.2(b) in Section 3.2. Therefore, the case with $m = 8$ and model=2(b) gives the optimal design in this example. Its parent design is 8-4.5, which includes columns 1, 2, 3, 4, 5, 6, 8, and 9 in Table 3.5 of Section 3.5. Since the 2fi's of the optimal design are (6, 8) and (6, 9), we assign the common factor, baking time, to column 6 and randomly assign baking temperature and the amount of milk to columns 8 and 9. The rest of factors can be randomly assigned to columns 1, 2, 3, 4, and 5. Since the "relabeling" is "1, 6", the levels of columns 1 and 6 are interchanged. Using the above procedure, we can obtain the following design matrix.

Table 3.9: An Optimal Design for the Baking Example

Eggs	Powder	Flour	Sugar	Butter	Time	Temperature	Milk
1	2	3	4	5	6	8	9
1	0	1	0	1	0	0	1
1	0	1	0	1	0	1	0
1	0	1	1	0	1	0	1
1	0	1	1	0	1	1	0
1	1	0	0	1	1	0	1
1	1	0	0	1	1	1	0
1	1	0	1	0	0	0	1
1	1	0	1	0	0	1	0
0	0	0	0	0	0	0	0
0	0	0	0	0	0	1	1
0	0	0	1	1	1	0	0
0	0	0	1	1	1	1	1
0	1	1	0	0	1	0	0
0	1	1	0	0	1	1	1
0	1	1	1	1	0	0	0
0	1	1	1	1	0	1	1

Chapter 4

Conclusions

In this project, we consider the problem of selecting optimal baseline two-level designs when some two-factor interactions (2fi's) are important. We first introduce the baseline parameterization and contrast it with the orthogonal parameterization. Then, we review and interpret the A- and D- optimality criteria and the minimum K-aberration criterion proposed by Mukerjee and Tang (2012). Since Mukerjee and Tang (2012) considered how to select optimal baseline designs for main effect models, the minimum K-aberration criterion cannot be directly used when there are some important 2fi's in the model. We propose a modified criterion, the minimum Q-aberration criterion, for this purpose. We develop a new search algorithm based on the optimality criteria and the minimum Q-aberration criterion. One concern about our search algorithm is that the running time increases exponentially as the number m of factors increases because we can generate $2^m q$ designs from q combinatorially nonisomorphic designs. To reduce running time, we can consider using only the first few Q values rather than all $Q_2, \ldots, Q_m$ to compare different designs.

We present collections of optimal baseline two-level designs of 16 runs and 20 runs. For each case considered in the results of 16-run designs, all the competing designs are equally efficient. Thus, the optimal designs of 16 runs are actually the minimum Q-aberration designs. However, for 20-run designs, the D values and A values are not the same for all competing designs in each case. Therefore, the optimal designs of 20 runs are the minimum Q-aberration designs among the A-best (or D-best) designs. Moreover, the results are very similar no matter which optimality criterion we use for 20 runs. In a future study, we will consider developing an incomplete algorithm to search for optimal baseline designs of larger sizes when some 2fi's are important.

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Appendix A

Parent Designs of 20 Runs

For $m = 4$,

1	1	0	0
0	1	1	0
1	0	1	1
1	1	0	1
0	1	1	0
0	0	1	1
0	0	0	1
0	0	0	0
1	0	0	0
0	1	0	0
1	0	1	0
0	1	0	1
1	0	1	0
1	1	0	1
1	1	1	0
1	1	1	1
0	1	1	1
0	0	1	1
1	0	0	1
0	0	0	0

Design 1

For $m = 5$,

1	1	1	0	1
1	1	0	1	1
1	1	0	1	0
1	1	0	0	1
1	1	0	0	0
1	0	1	1	1
1	0	1	1	0
1	0	1	0	1
1	0	1	0	0
1	0	0	1	0
0	1	1	1	0
0	1	1	1	0
0	1	1	0	1
0	1	1	0	0
0	1	0	1	1
0	0	1	1	1
0	0	0	1	1
0	0	0	0	1
0	0	0	0	0
0	0	0	0	0

Design 5

1	1	1	1	0
1	1	1	0	1
1	1	0	1	1
1	1	0	0	1
1	1	0	0	0
1	0	1	1	0
1	0	1	0	1
1	0	1	0	0
1	0	0	1	1
1	0	0	1	0
0	1	1	1	0
0	1	1	0	1
0	1	1	0	0
0	1	0	1	1
0	1	0	1	0
0	0	1	1	1
0	0	1	1	1
0	0	0	0	1
0	0	0	0	0
0	0	0	0	0

Design 8

1	1	1	0	1
1	1	1	0	0
1	1	0	1	1
1	1	0	1	0
1	1	0	0	0
1	0	1	1	1
1	0	1	1	0
1	0	1	0	0
1	0	0	1	1
1	0	0	0	1
0	1	1	1	1
0	1	1	1	0
0	1	1	0	1
0	1	0	1	0
0	1	0	0	1
0	0	1	1	0
0	0	1	0	1
0	0	0	1	1
0	0	0	0	0
0	0	0	0	0

Design 10

For $m = 6$,

1	1	1	0	1	0
1	1	0	1	1	1
1	1	0	1	0	1
1	1	0	0	1	1
1	1	0	0	0	0
1	0	1	1	1	0
1	0	1	1	0	1
1	0	1	0	1	1
1	0	1	0	0	0
1	0	0	1	0	0
0	1	1	1	0	1
0	1	1	1	0	0
0	1	1	0	1	0
0	1	1	0	0	1
0	1	0	1	1	0
0	0	1	1	1	1
0	0	0	1	1	0
0	0	0	0	1	1
0	0	0	0	0	1
0	0	0	0	0	0

Design 46

1	1	1	0	1	1
1	1	0	1	1	0
1	1	0	1	0	0
1	1	0	0	1	1
1	1	0	0	0	0
1	0	1	1	1	0
1	0	1	1	0	1
1	0	1	0	1	1
1	0	1	0	0	0
1	0	0	1	0	1
0	1	1	1	0	1
0	1	1	1	0	0
0	1	1	0	1	0
0	1	1	0	0	1
0	1	0	1	1	1
0	0	1	1	1	0
0	0	0	1	1	1
0	0	0	0	1	0
0	0	0	0	0	1
0	0	0	0	0	0

Design 47

1	1	1	0	1	1
1	1	0	1	1	0
1	1	0	1	0	1
1	1	0	0	1	0
1	1	0	0	0	0
1	0	1	1	1	1
1	0	1	1	0	0
1	0	1	0	1	0
1	0	1	0	0	1
1	0	0	1	0	1
0	1	1	1	0	1
0	1	1	1	0	0
0	1	1	0	1	1
0	1	1	0	0	0
0	1	0	1	1	1
0	0	1	1	1	0
0	0	0	1	1	0
0	0	0	0	1	1
0	0	0	0	0	1
0	0	0	0	0	0

Design 57

1	1	1	0	0	1
1	1	0	1	1	1
1	1	0	1	0	0
1	1	0	0	1	1
1	1	0	0	0	0
1	0	1	1	1	1
1	0	1	1	0	1
1	0	1	0	1	0
1	0	1	0	0	0
1	0	0	1	1	0
0	1	1	1	0	1
0	1	1	1	0	0
0	1	1	0	1	1
0	1	1	0	1	0
0	1	0	1	1	0
0	0	1	1	1	0
0	0	0	1	0	1
0	0	0	0	1	1
0	0	0	0	0	1
0	0	0	0	0	0

Design 58

1	1	1	1	0	1
1	1	1	0	1	1
1	1	0	1	1	0
1	1	0	0	1	1
1	1	0	0	0	0
1	0	1	1	0	1
1	0	1	0	1	0
1	0	1	0	0	0
1	0	0	1	1	1
1	0	0	1	0	0
0	1	1	1	0	0
0	1	1	0	1	0
0	1	1	0	0	1
0	1	0	1	1	0
0	1	0	1	0	1
0	0	1	1	1	1
0	0	1	1	1	0
0	0	0	0	1	1
0	0	0	0	0	1
0	0	0	0	0	0

Design 67

1	1	1	1	0	1
1	1	1	0	1	0
1	1	0	1	1	0
1	1	0	0	1	1
1	1	0	0	0	0
1	0	1	1	0	0
1	0	1	0	1	1
1	0	1	0	0	0
1	0	0	1	1	1
1	0	0	1	0	1
0	1	1	1	0	0
0	1	1	0	1	1
0	1	1	0	0	1
0	1	0	1	1	0
0	1	0	1	0	1
0	0	1	1	1	1
0	0	1	1	1	0
0	0	0	0	1	0
0	0	0	0	0	1
0	0	0	0	0	0

Design 69

1	1	1	1	0	1
1	1	1	0	1	1
1	1	0	1	1	1
1	1	0	0	1	0
1	1	0	0	0	0
1	0	1	1	0	0
1	0	1	0	1	1
1	0	1	0	0	0
1	0	0	1	1	0
1	0	0	1	0	1
0	1	1	1	0	0
0	1	1	0	1	0
0	1	1	0	0	1
0	1	0	1	1	0
0	1	0	1	0	1
0	0	1	1	1	1
0	0	1	1	1	0
0	0	0	0	1	1
0	0	0	0	0	1
0	0	0	0	0	0

Design 70

For $m = 7$,

1	1	1	0	1	0	1
1	1	0	1	1	1	0
1	1	0	1	1	0	1
1	1	0	0	0	1	1
1	1	0	0	0	0	0
1	0	1	1	0	1	0
1	0	1	1	0	0	1
1	0	1	0	1	1	1
1	0	1	0	0	1	0
1	0	0	1	1	0	0
0	1	1	1	0	1	1
0	1	1	1	0	0	0
0	1	1	0	1	1	0
0	1	1	0	1	0	0
0	1	0	1	0	1	1
0	0	1	1	1	0	1
0	0	0	1	1	1	0
0	0	0	0	1	1	1
0	0	0	0	0	0	1
0	0	0	0	0	0	0

Design 90

1	1	1	0	1	0	1
1	1	0	1	1	0	0
1	1	0	1	0	1	0
1	1	0	0	1	1	1
1	1	0	0	0	0	0
1	0	1	1	1	0	1
1	0	1	1	0	1	0
1	0	1	0	1	1	0
1	0	1	0	0	0	1
1	0	0	1	0	1	1
0	1	1	1	0	1	1
0	1	1	1	0	0	0
0	1	1	0	1	1	0
0	1	1	0	0	1	1
0	1	0	1	1	0	1
0	0	1	1	1	0	0
0	0	0	1	1	1	1
0	0	0	0	1	1	0
0	0	0	0	0	0	1
0	0	0	0	0	0	0

Design 334

1	1	1	0	1	1	0
1	1	0	1	1	1	1
1	1	0	1	0	0	0
1	1	0	0	1	0	1
1	1	0	0	0	1	1
1	0	1	1	1	0	0
1	0	1	1	0	0	1
1	0	1	0	1	0	1
1	0	1	0	0	1	0
1	0	0	1	0	1	0
0	1	1	1	0	1	0
0	1	1	1	0	0	1
0	1	1	0	1	0	0
0	1	1	0	0	1	1
0	1	0	1	1	0	0
0	0	1	1	1	1	1
0	0	0	1	1	1	1
0	0	0	0	1	1	0
0	0	0	0	0	0	1
0	0	0	0	0	0	0

Design 403

1	1	1	0	1	1	1
1	1	0	1	1	1	1
1	1	0	1	0	1	0
1	1	0	0	1	0	1
1	1	0	0	0	0	0
1	0	1	1	1	0	0
1	0	1	1	0	1	0
1	0	1	0	1	1	0
1	0	1	0	0	0	1
1	0	0	1	0	0	1
0	1	1	1	0	1	1
0	1	1	1	0	0	1
0	1	1	0	1	0	0
0	1	1	0	0	1	0
0	1	0	1	1	0	0
0	0	1	1	1	0	1
0	0	0	1	1	1	0
0	0	0	0	1	1	1
0	0	0	0	0	1	1
0	0	0	0	0	0	0

Design 425

1	1	1	0	1	1	1
1	1	0	1	1	1	1
1	1	0	1	0	1	0
1	1	0	0	1	0	0
1	1	0	0	0	0	1
1	0	1	1	1	0	0
1	0	1	1	0	1	0
1	0	1	0	1	1	0
1	0	1	0	0	0	1
1	0	0	1	0	0	1
0	1	1	1	0	1	1
0	1	1	1	0	0	0
0	1	1	0	1	0	1
0	1	1	0	0	1	0
0	1	0	1	1	0	0
0	0	1	1	1	0	1
0	0	0	1	1	1	1
0	0	0	0	1	1	0
0	0	0	0	0	1	1
0	0	0	0	0	0	0

Design 429

1	1	1	0	1	0	1
1	1	0	1	1	1	0
1	1	0	1	0	1	1
1	1	0	0	1	1	1
1	1	0	0	0	0	0
1	0	1	1	1	0	0
1	0	1	1	0	1	0
1	0	1	0	1	1	0
1	0	1	0	0	0	1
1	0	0	1	0	0	1
0	1	1	1	0	1	1
0	1	1	1	0	0	0
0	1	1	0	1	0	1
0	1	1	0	0	1	0
0	1	0	1	1	0	0
0	0	1	1	1	1	1
0	0	0	1	1	0	1
0	0	0	0	1	1	0
0	0	0	0	0	1	1
0	0	0	0	0	0	0

Design 430

1	1	1	0	1	1	0
1	1	0	1	1	0	0
1	1	0	1	0	0	1
1	1	0	0	1	1	1
1	1	0	0	0	0	0
1	0	1	1	1	1	1
1	0	1	1	0	0	1
1	0	1	0	1	0	0
1	0	1	0	0	1	1
1	0	0	1	0	1	0
0	1	1	1	0	1	0
0	1	1	1	0	1	0
0	1	1	0	1	0	1
0	1	1	0	0	0	1
0	1	0	1	1	1	1
0	0	1	1	1	0	0
0	0	0	1	1	0	1
0	0	0	0	1	1	0
0	0	0	0	0	1	1
0	0	0	0	0	0	0

Design 451

1	1	1	1	0	1	0
1	1	1	0	1	1	1
1	1	0	1	1	0	0
1	1	0	0	1	1	0
1	1	0	0	0	0	1
1	0	1	1	0	1	1
1	0	1	0	1	0	0
1	0	1	0	0	0	1
1	0	0	1	1	1	1
1	0	0	1	0	0	0
0	1	1	1	0	0	0
0	1	1	0	1	0	1
0	1	1	0	0	1	0
0	1	0	1	1	0	1
0	1	0	1	0	1	1
0	0	1	1	1	1	0
0	0	1	1	1	0	1
0	0	0	0	1	1	0
0	0	0	0	0	1	1
0	0	0	0	0	0	0

Design 471